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SUPPLEMENTARY INFORMATION

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Selective molecular recognition by nanoscale environments in a supported iridium cluster catalyst

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Figures and Tables

Materials and Methods

Synthesis and characterization of cluster compounds **1** and **2** have been previously described.(Reference *12* in the manuscript)

Preparation of ***SiO_2-500***

Aerosil 200 was kindly provided by Evonik Industries AG. Ten grams of Aerosil 200 were mixed with 200 mL nanopure water. The mixture was heated at 120 °C under vigorous stirring for 24 h. After the mixture was cooled to room temperature, the slurry was centrifuged and the water phase was decanted. The solid was dried at 200 °C for 15 h under vacuum. After cooling to room temperature, the solid material was thoroughly crushed with mortar and pestle. The obtained powder was then treated in a flow bed reactor as followed: flow of dry air (110 mL/min) and argon (55 mL / min), temperature program: 5° C/min ramp to 95 °C, soak for 20 min, 5 °C/min ramp to 500 °C, soak 4 h, turn off dry air flow, lower argon flow to 15 ml / min, hold 500 °C for 10 h, cool to room temperature. The powder was then stored in vials in a glove box under argon atmosphere.

Preparation of ***1-SiO_2-500***

A solution of 51 mg (0.013 mmol) cluster **1** in 3 mL freshly distilled hexane was added to slurry of 949 mg **SiO_2-500** and 20 mL hexane. The mixture was stirred for 1 h and the hexane was evaporated. The remaining powder was dried under vacuum at room temperature for 0.5 h.

Preparation of ***3-SiO_2-500 and 4-SiO_2-500***

Synthesis of ***3-SiO_2-500*****:** To a solution of 51 mg (0.013 mmol) cluster **1** was added 100 μL of a solution of 100 mg (1.33 mmol) Me_3NO in 10 mL dichloromethane. The solution color changed immediately from yellow to brown. The solution was stirred for 1 h and added to slurry of 949 mg **SiO_2-500** and 20 mL hexane. The mixture was stirred for 1 h and the hexane was evaporated. The remaining powder was dried under vacuum at room temperature for 0.5 h.

Synthesis of ***4-SiO_2-500*****:** To a solution of 51 mg (0.013 mmol) cluster **1** was added 195 μL of a solution of 100 mg (1.33 mmol) Me_3NO in 10 mL dichloromethane. The solution color changed immediately from yellow to brown. The solution was stirred for 1 h and added to slurry of 949 mg **SiO_2-500** and 20 mL hexane. The mixture was stirred for 1 h and the hexane was evaporated. The remaining powder was dried under vacuum at room temperature for 0.5 h.

We investigated recarbonylation of the supported open clusters **3-SiO_2-500** and **4-SiO_2-500**, and the data are summarized in Table S1. Both of these supported clusters were recarbonylated to an extent corresponding to approximately 50% of that observed for the unsupported clusters in decane solution. The difference cannot be ascribed to remaining trimethylamine because it was removed during evacuation of supported catalysts (vide supra). IR data (see Figure S8) show that treatment of **3-SiO_2-500** and **4-SiO_2-500** with CO resulted in gradual recarbonylation over 40 h. This observation is in contrast to the complete recarbonylation in 2 h of the corresponding open clusters in decane solution. The slowing of the recarbonylation and the decrease in

recarbonylation capacity observed for the supported clusters cannot be ascribed to mass transport restrictions, because recarbonylation of supported clusters (such as shown in Figure 3a) can intrinsically occur much faster. Instead, we attribute the observations to the influence of the silica support acting as a competitive ligand - blocking open sites from recarbonylation, even though silica is a support that is expected to minimize such interactions. Similar support effects may account for previous observations of partial recarbonylation - recarbonylation of fully decarbonylated Ir_4 clusters supported on partially dehydroxylated MgO led to only 13% of the open sites being recarbonylated (*S1, S2*). The results summarized above demonstrate that CO can access open sites on the supported clusters.

*Decarbonylation and recarbonylation of cluster **1** using 1 equivalent of Me_3NO in solution*

To a solution of 51 mg (0.013 mmol) cluster **1** in 3 mL decane was added 100 μL of a solution of 100 mg (1.33 mmol) Me_3NO in 10 mL dichloromethane. The solution color changed immediately from yellow to brown. After 1h, the head space of the schlenk flask was evacuated and purged with CO gas. The color of the solution immediately changed from brown to yellow. Samples for DLS, NMR and FTIR spectroscopy were taken before Me_3NO addition, after Me_3NO addition, and after CO treatment. In addition to DLS data mentioned in the manuscript, which shows lack of cluster aggregation for **3** and **4**, we monitored the reactive decarbonylation process using TMAO via ^{1}H NMR spectroscopy with the sample in C_6D_{12} solution. Although the ^{1}H NMR spectra of **3** and **4** did not change during decarbonylation, which is yet another indication of retention of cluster stability, a new resonance appeared at 2.14 ppm, which is assigned to bound Me_3N (we measured the chemical shift of Me_3N via ^{1}H NMR in the same solvent as the experiment at 2.12 ppm, which is consistent with the previously assigned ^{1}H NMR Me_3N resonance (*41*). Such a small shift of bound versus free Me_3N is expected on the basis of previous measurements of trimethylamine coordinated to neutral tetrahedral metal carbonyl clusters. (*42*) Me_3N was removed (verified by absence of resonance in the ^{1}H NMR spectrum) by evacuating **3** (for 15 h) and **4** (for 0.5 h) at 10 Pa at room temperature after synthesis. This result means that the final state of anchored clusters **3** and **4** on a silica support consists of CO vacancies, rather than bound Me_3N, since these clusters were similarly evacuated after anchoring

*Decarbonylation and recarbonylation of cluster **1** using 2 equivalents of Me_3NO in solution*

To a solution of 51 mg (0.013 mmol) cluster **1** in 3 mL decane was added 195 μL of a solution of 100 mg (1.33 mmol) Me_3NO in 10 mL dichloromethane. The solution color changed immediately from yellow to brown. After 1 h, the head space of the Schlenk flask was evacuated and purged with CO gas. The color of the solution immediately changed from brown to yellow. Samples for DLS, NMR and FTIR spectroscopy were taken before Me_3NO addition, after Me_3NO addition, and after CO treatment.

*Decarbonylation and recarbonylation of cluster **2** using 1 equivalent of Me_3NO in solution*

To a solution of 12 mg (0.007 mmol) cluster **1** in 2 mL decane was added 55 μL of a solution of 100 mg (1.33 mmol) Me_3NO in 10 mL dichloromethane. The solution color changed immediately from yellow to brown and the formation of a brown solid was observed. After 1 h, the head space of the Schlenk flask was evacuated and purged with CO gas. Samples for DLS,

NMR and FTIR spectroscopy were taken before Me_3NO addition, after Me_3NO addition, and after CO treatment.

Analysis of liquid samples

Infrared spectroscopy in solution was performed on a Bruker Tensor instrument using a liquid cell (CaF_2 windows, d = 0.5 mm). ^1H and $^{31}P\{^1H\}$-NMR spectra in solution were recorded in either decane-d_{12} or cyclohexane-d_{12} (20 ˚C), using either a Bruker AV-600 (600 MHz) instrument, an AVQ-400 (400 MHz), or an AVB-400 (400 Mhz) instrument at the UC Berkeley College of Chemistry NMR Facility. ^{31}P NMR data were referenced relative to trimethyl phosphate. ^1H-NMR data were referenced to Tetramethylsilane ($\delta = 0$ ppm). DLS was performed on a Malvern Nano-Zetasizer in glass cuvettes at 25 °C. Solvents were filtered through 0.02 μm filters prior use. Samples were given sufficient time to equilibrate to 25 °C. The results from at least four measurements are averaged and the number-average particle size values are reported.

*Liquid phase FTIR studies of ethylene bound **1** and **3***

250 mg **1-SiO_2-500** were washed with 4 x 1 mL toluene-d_8. The eluents were combined and treated with ethylene gas (30 sec bubbled through the solution at room temperature). FTIR spectra were recorded before and after ethylene treatment.
A solution of **3** in toluene-d_8 was treated with ethylene gas (30 sec bubbled through the solution at room temperature). FTIR spectra were recorded before and after ethylene treatment.
A solution of **3** in toluene was treated with ethylene-d_4 gas (30 sec bubbled through the solution at room temperature). FTIR spectra were recorded before and after ethylene treatment.

STEM

In the STEM experiments, to minimize the exposure to air and moisture, powder samples were loaded onto a lacey carbon, 300-mesh copper grid (Ted-Pella) in the glovebox. The grid in the glovebox was packed in an Eppendorf tube and sealed with Parafilm. Each Eppendorf tube was placed in a Swagelok stainless-steel tube sealed with O-rings for transfer to the microscope. There, an argon-filled glovebag (Glas-Col) was purged five times with ultrahigh purity argon, and the grid was loaded onto the sample holder in the glovebag under a blanket of flowing argon. As argon flowed over the sample holder, it was transferred from the glovebag to the microscope with an air exposure of at most 4 s. Images were obtained with a JEOL JEM-2100F electron microscope at the University of California, Davis. The microscope is equipped with an FEG, operated at 200 kV, with a CEOS hexapole probe (STEM) aberration corrector. The images were captured by a high-angle annular dark-field (HAADF) detector with a collection semi-angle of 75–200 mrad and a probe convergence semi-angle of 17.1 mrad. The imaging dose was approximately 10^5 $e^-/Å^2$. Prior to imaging of the samples, the aberration corrector was aligned with a Pt/Ir on holey carbon standard sample (SPI supplies) until atomic resolution of the metals was achieved and the lattice spacings of the metals were confirmed. Images (512 x 512 pixel size) were acquired with Digital Micrograph software (Gatan) in <5 s including instrument optimization on a neighboring region prior to image acquisition, minimizing the occurrence of electron beam damage. A total of approximately 30 clusters were analyzed for size measurement

on each set of samples. The average cluster diameter is reported with a standard deviation for the population of clusters analyzed. For each cluster, an intensity profile was obtained by using the Digital Micrograph software (Gatan). Line profiles were then transferred to OriginPro for baseline correction. Background-subtracted profiles of the clusters were fitted to a Gaussian distribution function in OriginPro, and FWHM values of the fitted peak are reported as the diameter of each cluster metal framework as illustrated previously (see C. Aydin, J. Lu, M. Shirai, N. D. Browning, B. C. Gates, *ACS Catal.* 1,1613–1620 (2011)**).** Accordingly, the mean diameter and the standard deviation for each sample are reported.

Solid state ^{31}P NMR spectroscopy

The solid-state cross polarization magic-angle-spinning nuclear magnetic resonance (CPMAS-NMR) measurements were performed using a Bruker Avance 500 MHz spectrometer with a wide bore 11.7 T magnet and using a Bruker 4 mm CPMAS probe. The resonance frequencies were 500.2 MHz and 202.5 MHz for proton (^{1}H) and phosphorous (^{31}P) nuclei, respectively. The samples were packed into a 4mm ZrO_2 rotor (Bruker) in an argon atmosphere glove box and sealed with a tight fitting kel-F cap (Bruker). Dry nitrogen gas was used for sample spinning in order to minimize oxidation from moisture or air contact. All ^{31}P CPMAS spectra reported here were acquired with cross polarization contact time of 2 ms under a sample spinning rate of 14 kHz. ^{31}P chemical shifts were referenced to concentrated phosphoric acid (H_3PO_4) ($\delta = 0.00$ ppm) externally.

BET surface area measurements

BET surface area measurements were collected by using a Micromeritics ASAP2020 at 77 K. Prior to measurement, samples were evacuated for 4 h at 313 K for **1-SiO_2-500** and at 523 K for **SiO_2-500** (support alone). The as-received silica (Degussa, Aerosil 200) has a reported surface area of 200 m^2/g. After hydration and calcination procedures, the **SiO_2-500** support was characterized by a surface area of 190 m^2/g. As-made **1-SiO_2-500** was characterized by a surface area of 170 m^2/g showing slightly reduced surface area as expected after cluster deposition.

Elemental analysis

ICP-OES elemental analysis on supported cluster **1-SiO_2-500** was performed by Intertek Pharmaceutical Services and was reported to contain 1.07 wt% Ir – within experimental uncertainty of expected value of 1.0 wt% Ir based on synthesis.

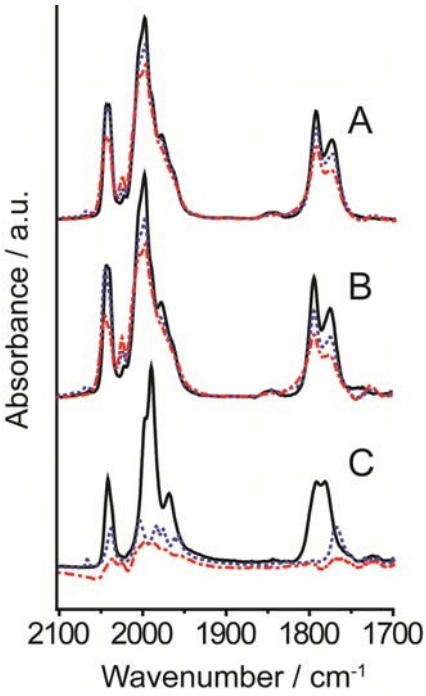


Fig. S1. IR spectroscopy of decane solutions of (A) **1** (black solid line), **3** (red dashed-dotted line), and recarbonylated **3** after CO treatment (blue dashed line); (B) **1** (black solid line), **4** (red dashed-dotted line), and recarbonylated **4** after CO treatment (blue dashed line); (C) **2** (black solid line), **2** following treatment with TMAO to give a nanoparticle aggregate (red dashed-dotted line), and nanoparticle aggregate representing **2** after TMAO and subsequent CO treatment (blue dashed line).

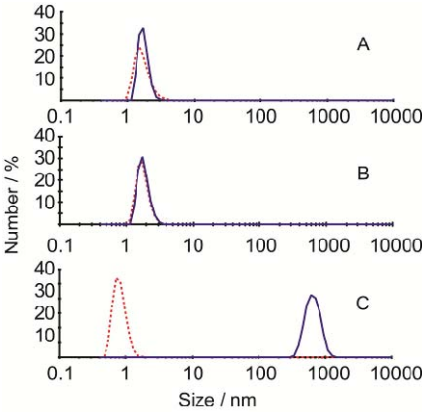


Fig. S2. Size distribution according to dynamic light scattering for 4.3 μM decane solutions of (A) **1** (red-dashed line), **3** (blue-solid line); (B) **1** (red-dashed line), **4** (blue-solid line); (C) **2** (red-dashed line), **2** following TMAO treatment (blue-solid line).

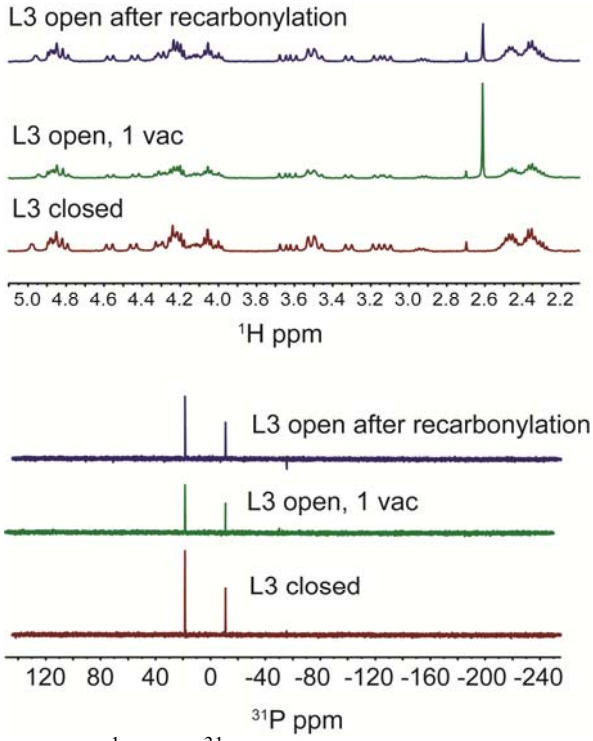


Fig. S3. ^{1}H and ^{31}P NMR data for clusters **1** (bottom), **3** (middle), and **3** after recarbonylation (top).

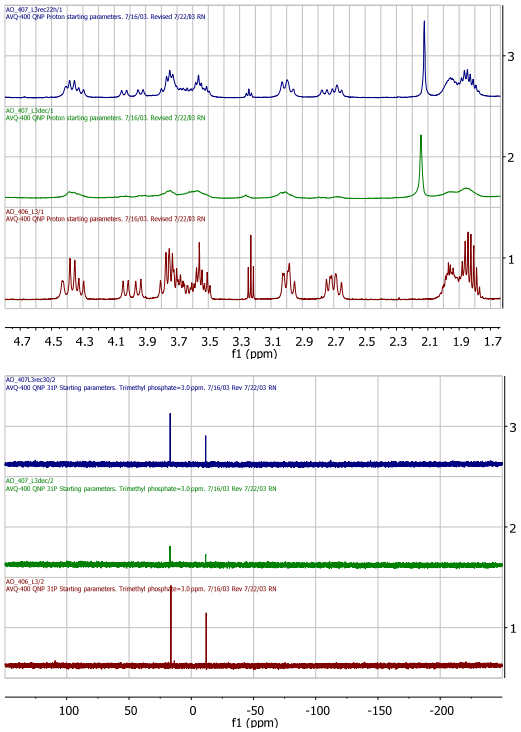


Fig. S4. ^{1}H and ^{31}P NMR data for clusters **1** (bottom), **4** (middle), and **4** after recarbonylation (top).

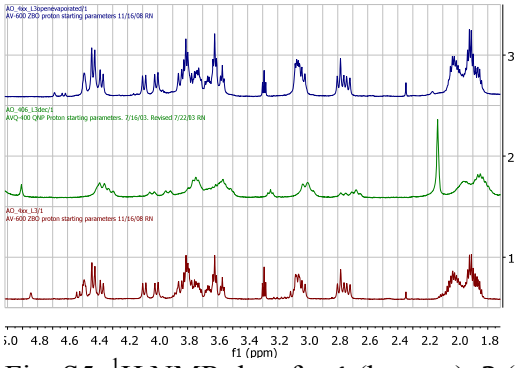


Fig. S5. ^{1}H NMR data for **1** (bottom), **3** (middle) and **3** after 15 h vacuum treatment (top)

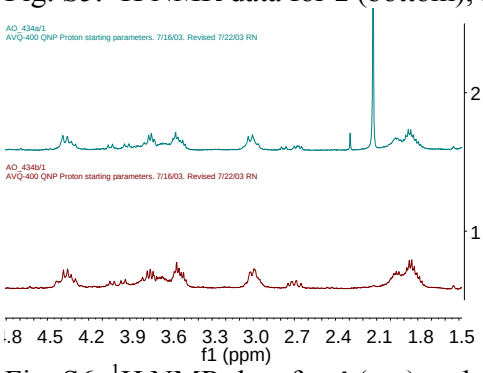


Fig. S6. ^{1}H NMR data for **4** (top) and **4** after 30 min vacuum treatment (bottom)

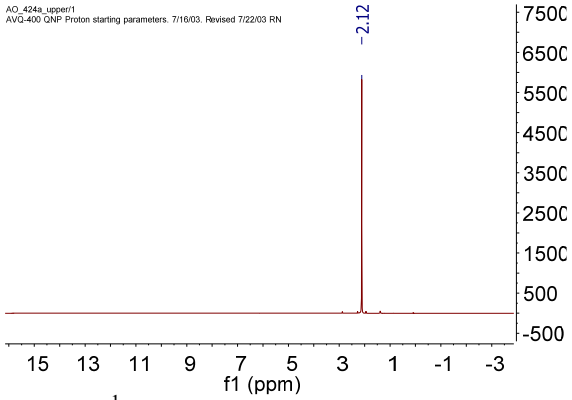


Fig. S7. ^{1}H NMR data for Me_3N in cyclohexane-d_{12}

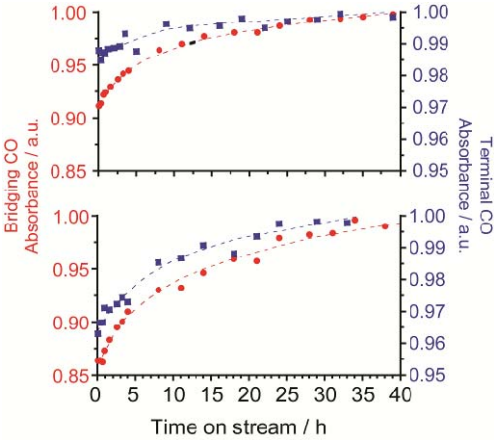


Fig. S8. CO absorbance intensity corresponding to bridging (red circles) and terminal (blue squares) CO bands as measured during recarbonylation of **3-SiO$_2$-500** (top) and **4-SiO$_2$-500** (bottom) using in-situ solid-state IR spectroscopy. During the experiment, a mixture of CO and helium flowed at 1 and 50 mL(NTP)/min, respectively, for 40 h, while the IR cell temperature was held at room temperature (approximately 23 °C). A value of 1.0 was arbitrarily assigned to the absorbance intensity (measured at the maximum) after 40 h of CO treatment.

Table S1. Characterization of supported cluster samples **3-SiO$_2$-500** and **4-SiO$_2$-500** using IR carbonyl-band absorbance intensities[b] after recarbonylation

Sample	# (CO) gained[a]	CO_{term} / %	CO_{bridg} / %
3-SiO$_2$-500 (recarb)	0.3	93	80
4-SiO$_2$-500 (recarb)	0.5	90	63

[a] # = number of CO molecules gained during recarbonylation per Ir_4 cluster

[b] Absorbance intensities were measured at 1994 cm^{-1} for terminal CO ligands and at 1784 cm^{-1} for bridging CO ligands and were normalized to the Si-O-Si peak at 1868 cm^{-1}. The reported relative intensities are reported as a % relative to corresponding normalized CO-band absorbance intensity in **1-SiO$_2$-500**.

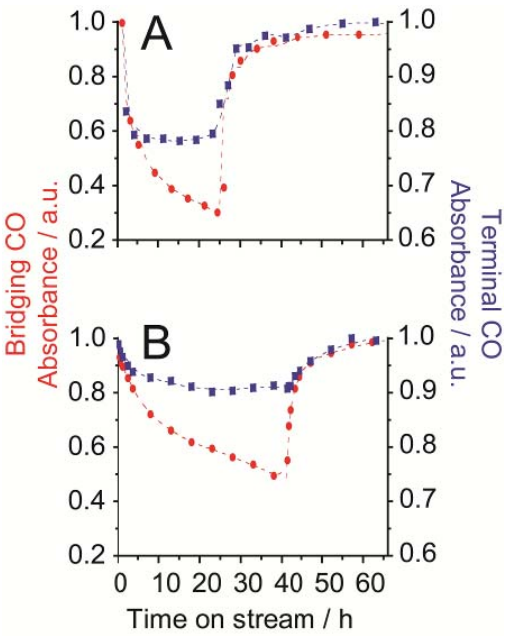


Fig. S9. Integrated CO intensity corresponding to bridging (red circles) and terminal (blue squares) CO bands as measured during ethylene hydrogenation catalysis followed by recarbonylation via CO treatment, using in-situ FTIR spectroscopy of (A) **1-SiO_2-500** and (B) **3-SiO_2-500**. The data demonstrate significant loss of carbonyl ligands from each catalyst during ethylene hydrogenation catalysis in the presence of the flowing gases. For each catalyst, the decarbonylation was found to be reversible by subsequent treatments in CO. Catalysis conditions were 40 °C, ambient pressure, and total flow rate of 63 mL/min (NTP) (16% H_2, 5% C_2H_4, balance He) for (A) 24 h and (B) 40 h. Subsequently, a mixture of CO and He flowed at 1 and 50 mL/min (NTP), respectively, for (A) 40 h and (B) 24 h, while the IR cell temperature was held at room temperature (approximately 23 °C). Measured intensities for all samples after recarbonylation were arbitrarily set to 1.0. These data imply the lack of a direct correlation between catalytic activity and the number of CO vacancies created on a metal cluster by decarbonylation in flowing gas. Although most CO ligands had been removed during 25 h of ethylene hydrogenation catalyzed by **1-SiO_2-500**, the activity of this catalyst was found to be much less than that of **3-SiO_2-500**–because in the presence of the flowing gas, CO vacancies are created within selective nanoenvironments where ethylene does not bind.

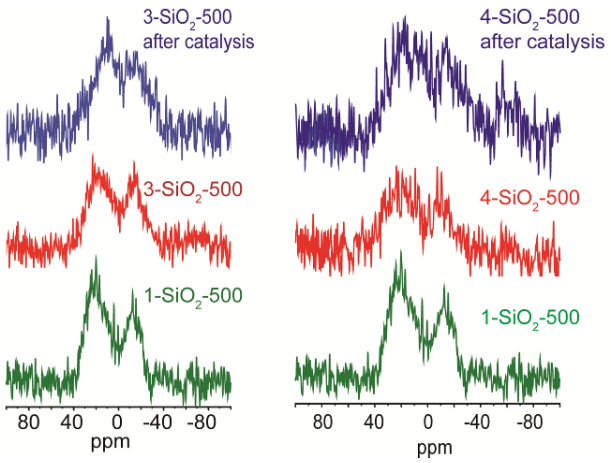
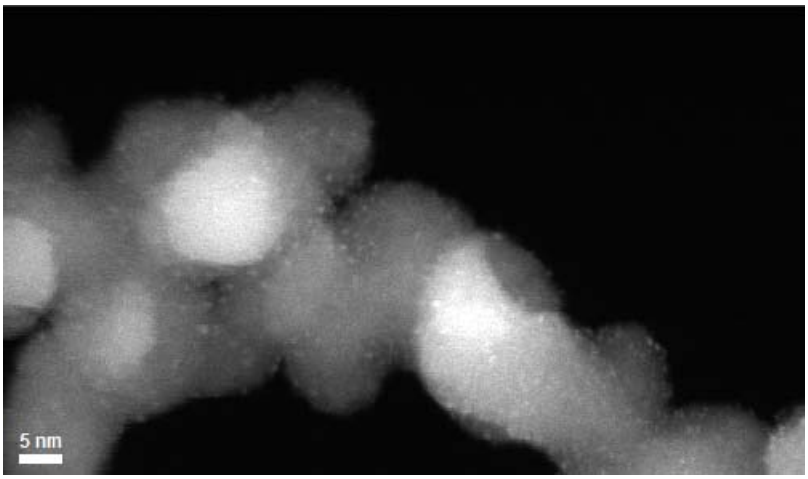
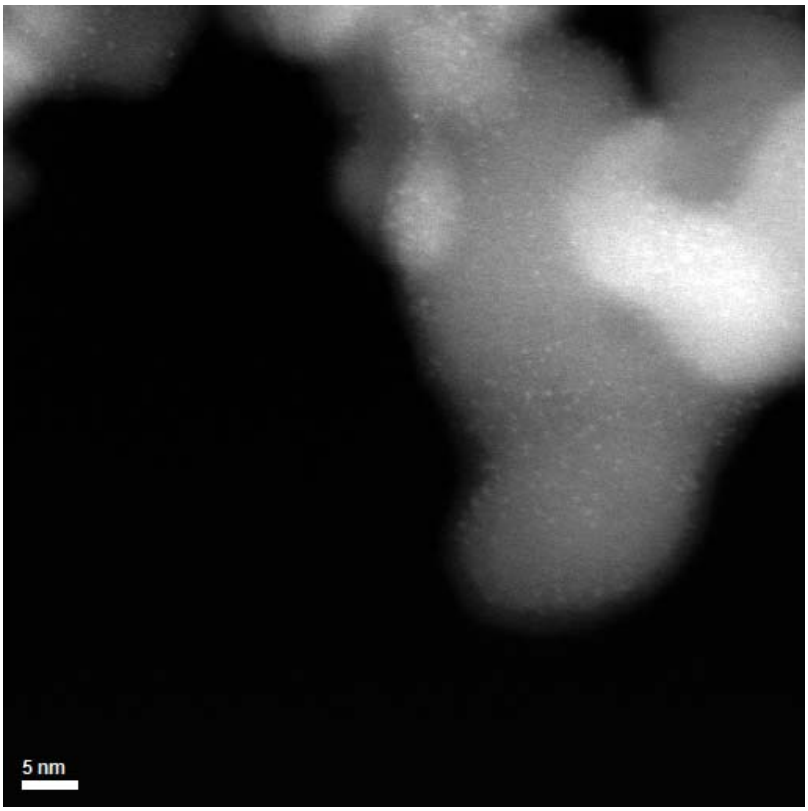


Fig. S10. ^{31}P CPMAS NMR data of **1-SiO$_2$-500** (green, bottom, left and right), **3-SiO$_2$-500** before catalysis (red, middle left), **3-SiO$_2$-500** after catalysis (blue, top left) **4-SiO$_2$-500** before catalysis (red, middle right), **4-SiO$_2$-500** after catalysis (blue, top right).





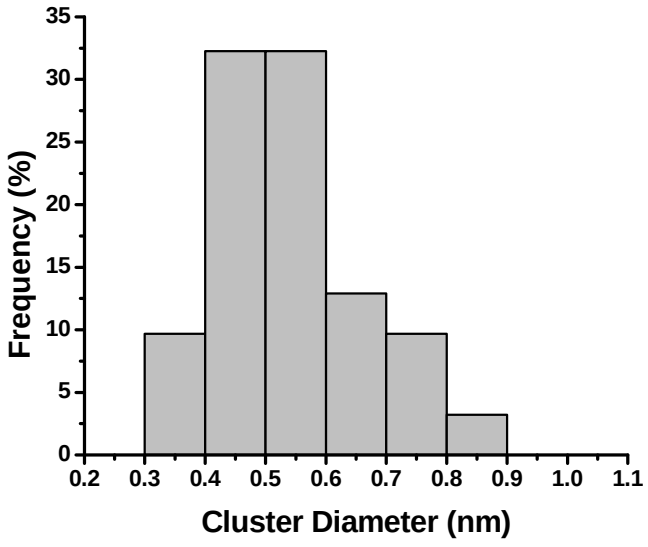
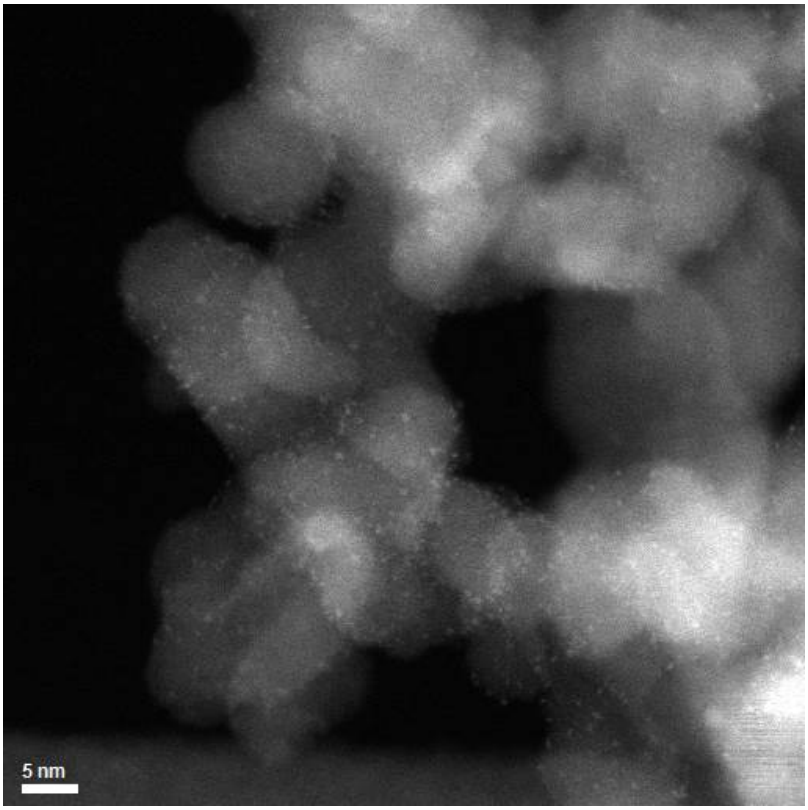
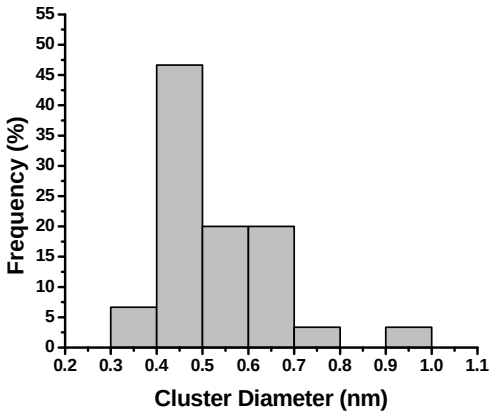


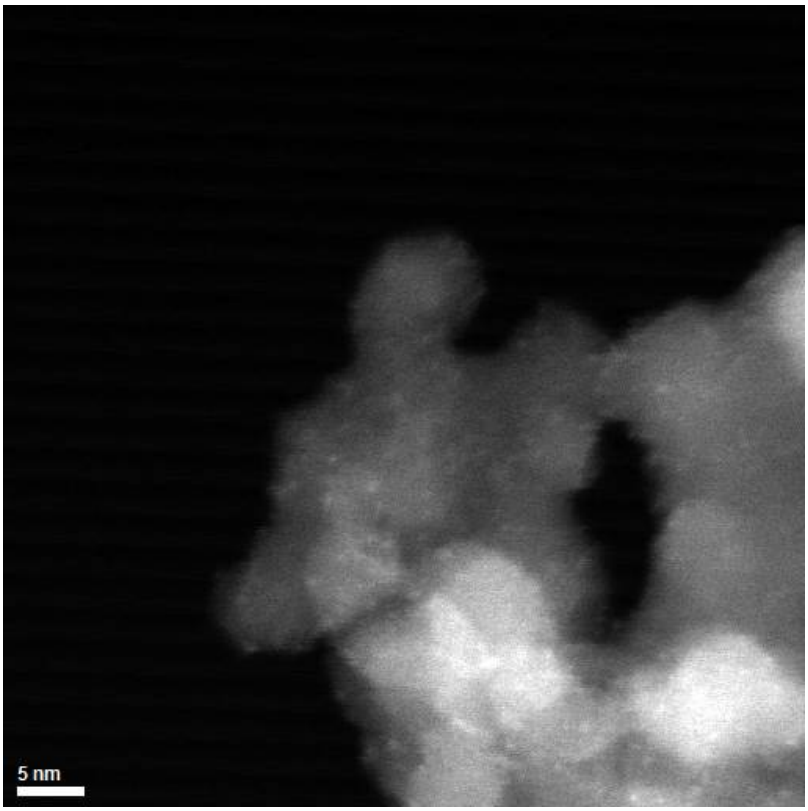
Fig. S11. HAADF-STEM images and histogram showing the distribution of nanocluster diameters characterizing the sample incorporating silica-supported iridium species **3-SiO_2-500**. The STEM data are consistent with the lack of cluster aggregation. The data demonstrate that the cluster size has not changed as a result of the oxidative treatment or the subsequent C_2H_4 hydrogenation catalysis, because the measured diameter matches that previously reported for a sphere tightly encapsulating the Ir_4 tetrahedron in $Ir_4(CO)_{12}$, calculated based on crystallographic data (see D. Braga, F. Grepioni, J.J. Byrne, M.J. Calhorda, Journal of the Chemical Society, Dalton Transactions, 20 (1995)).

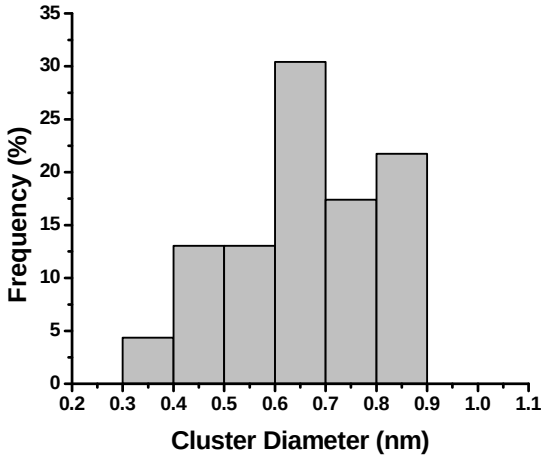




(Average: 0.53 ± 0.12 nm)

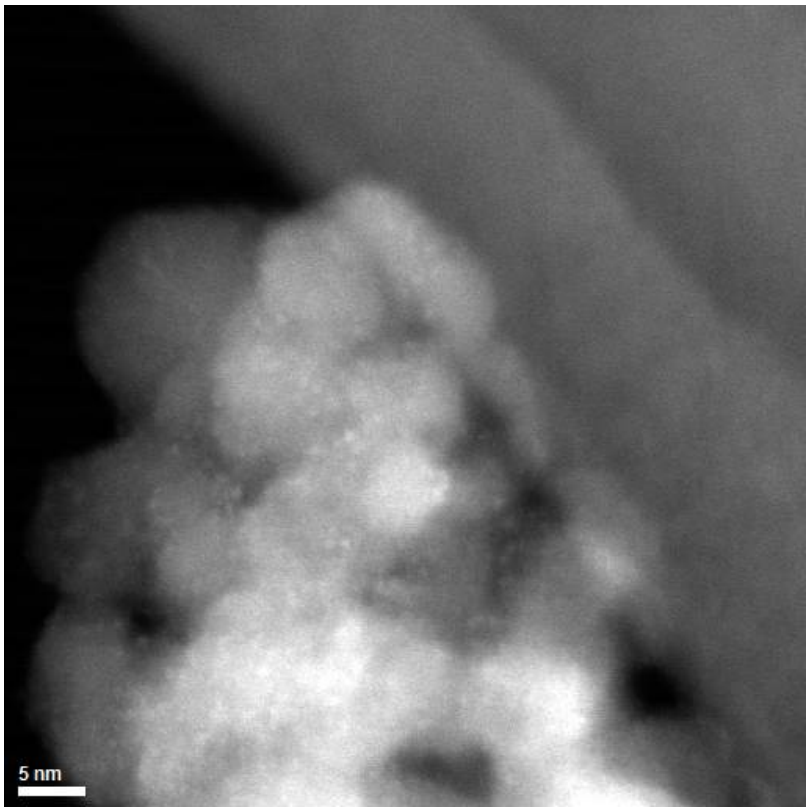
Fig. S12. HAADF-STEM images and histogram showing the distribution of nanocluster diameters characterizing the sample incorporating silica-supported iridium species **3-SiO_2-500** after ethylene hydrogenation at 40°C. The STEM data are consistent with the lack of cluster aggregation. The data demonstrate that the cluster size has not changed as a result of the oxidative treatment or the subsequent C_2H_4 hydrogenation catalysis, because the measured diameter matches that previously reported for a sphere tightly encapsulating the Ir_4 tetrahedron in $Ir_4(CO)_{12}$, calculated based on crystallographic data (see D. Braga, F. Grepioni, J.J. Byrne, M.J. Calhorda, Journal of the Chemical Society, Dalton Transactions, 20 (1995)).

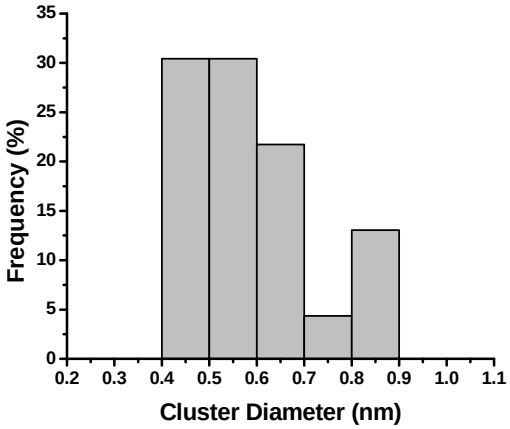




(Average: 0.65 ± 0.16 nm)

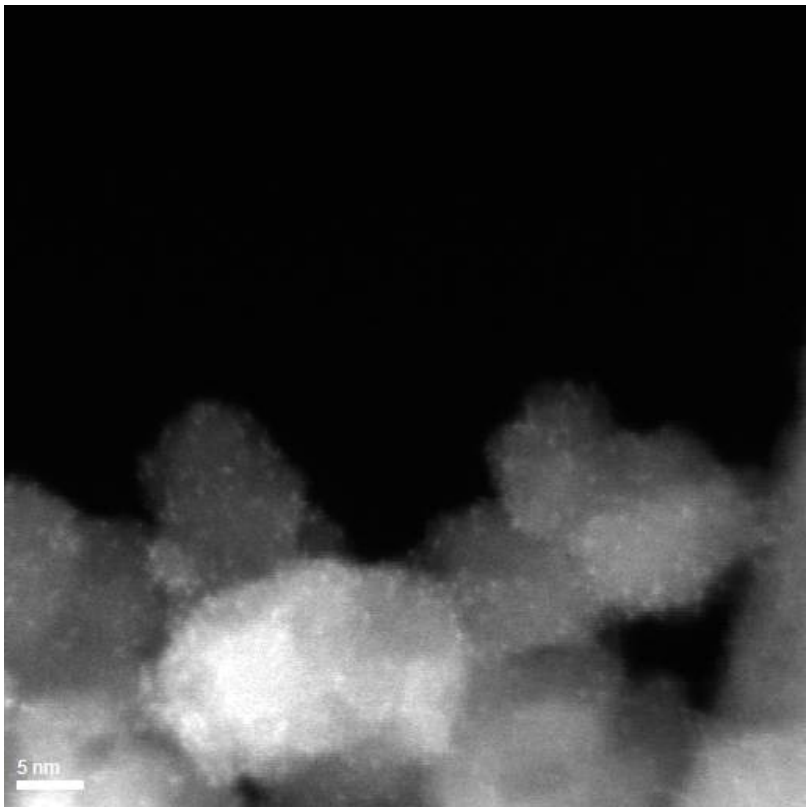
Fig. S13. HAADF-STEM images and histogram showing the distribution of nanocluster diameters characterizing the sample incorporating silica-supported iridium species **3-SiO_2-500** after ethylene hydrogenation at 50°C. The STEM data are consistent with the lack of cluster aggregation. The data demonstrate that the cluster size has not changed as a result of the oxidative treatment or the subsequent C_2H_4 hydrogenation catalysis, because the measured diameter matches that previously reported for a sphere tightly encapsulating the Ir_4 tetrahedron in $Ir_4(CO)_{12}$, calculated based on crystallographic data (see D. Braga, F. Grepioni, J.J. Byrne, M.J. Calhorda, Journal of the Chemical Society, Dalton Transactions, 20 (1995)).

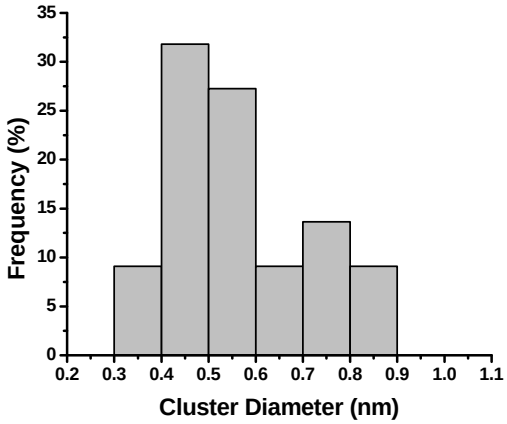




(Average: 0.60 ± 0.13 nm)

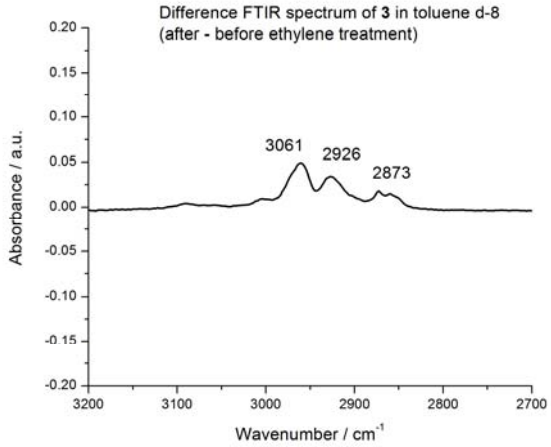
Fig. S14. HAADF-STEM images and histogram showing the distribution of nanocluster diameters characterizing the sample incorporating silica-supported iridium species **4-SiO_2-500**. The STEM data are consistent with the lack of cluster aggregation. The data demonstrate that the cluster size has not changed as a result of the oxidative treatment or the subsequent C_2H_4 hydrogenation catalysis, because the measured diameter matches that previously reported for a sphere tightly encapsulating the Ir_4 tetrahedron in $Ir_4(CO)_{12}$, calculated based on crystallographic data (see D. Braga, F. Grepioni, J.J. Byrne, M.J. Calhorda, Journal of the Chemical Society, Dalton Transactions, 20 (1995)).

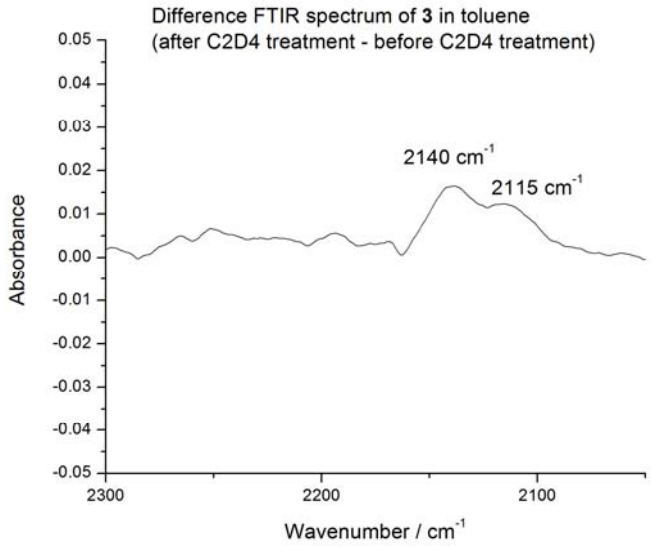




(Average: 0.55 ± 0.14 nm)

Fig. S15. HAADF-STEM images and histogram showing the distribution of nanocluster diameters characterizing the sample incorporating silica-supported iridium species **4-SiO_2-500** after ethylene hydrogenation at 40°C. The STEM data are consistent with the lack of cluster aggregation. The data demonstrate that the cluster size has not changed as a result of the oxidative treatment or the subsequent C_2H_4 hydrogenation catalysis, because the measured diameter matches that previously reported for a sphere tightly encapsulating the Ir_4 tetrahedron in $Ir_4(CO)_{12}$, calculated based on crystallographic data (see D. Braga, F. Grepioni, J.J. Byrne, M.J. Calhorda, Journal of the Chemical Society, Dalton Transactions, 20 (1995)).





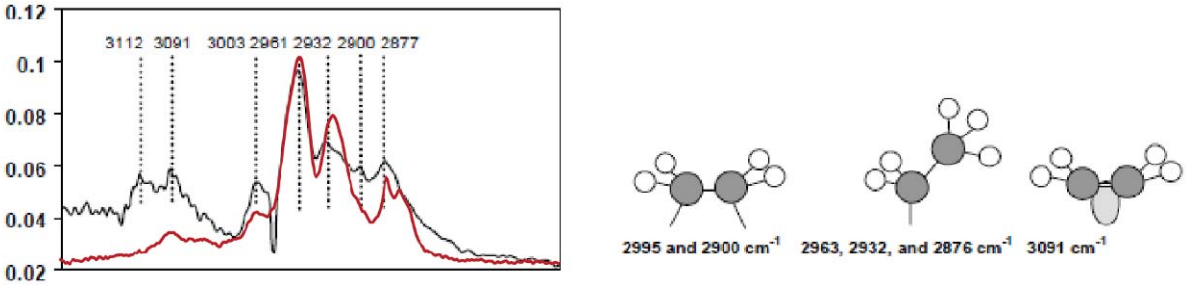


Figure S16. Top and middle: FTIR difference spectra of open cluster **3** after and before ethylene treatment in either toluene-d_8 (top panel) or toluene (middle panel). Bottom: comparison with band assignments for ethyl bound to Ir_4 cluster as previously reported ethyl IR bands (black line, Reference *17*) with data from this manuscript (red data). The complete overlap with previously

reported ethyl bands confirms that ethyl is bound to cluster 3 upon its treatment with ethylene gas. The assignments reported in the bottom panel are taken from Reference 17.

Table S2. Wavenumber and assignment of IR bands observed on **3-SiO_2-500** after ethylene treatment. (Assignment based on reference (*17*)

Adsorbate	Bands, cm^{-1}
di-σ-bonded ethylene	2990(s), 2985
Ethylidyne	2955, 2884
Ethyl	2965, 2935, 2884(s)

DFT calculations

Density functional theory (DFT) calculations were performed using the Gaussian 09[S3] package. An ONIOM [S4], quantum mechanics/molecular mechanics (QM/MM) approach was used for modeling the full-calixarene-phosphine system, due to the size of the calixarene substituent on the phosphine groups. The B3LYP [S5, S6] functional with a pseudopotential and split valence basis set was used for the quantum mechanical layer. The LANL2DZ [S7] basis set and pseudopotential was used for the iridium atoms and the all electron 6-31+G(d,p) basis set [S8- S10] was used for the main group species in the quantum mechanical layer. The molecular mechanics layer utilized the universal force field (UFF) [S11]. Selection of layers was based upon the proximity of the atoms to the active center. The Ir, P, C and O of the carbonyl groups and C, H of the ethylene and ethyl molecule are the atoms in the high level quantum mechanical layer.

Steric and electronic effects on the preferred reaction sites for ethylene and ethyl to the iridium cluster were tested by replacing the three PPh_2calixarene with three trimethylphosphine $(PMe_3)_3$. In this case, a full quantum mechanical DFT calculation with the functionals and basis sets given above was performed. All calculations were conducted in the gas phase at standard temperature and pressure (298.15 K and 1 atm).

Structures were optimized using density functional theory starting with the coordinates of **1** from single-crystal X-ray diffraction. The structures of ethyl and ethylene reaction at the various positions for the $(PPh_2Calixarene)_3$ and $(PMe_3)_3$ systems were fully optimized. The energies reported are ΔG of reaction in kcal/mol.

The reaction energies are calculated for the displacement of CO by the organic (equations 1 and 2) with L the phosphine ligand and R = C_2H_4, C_2H_5. For R = C_2H_5, the calcualtions are done for a doublet.

$$^{1}Ir_4CO_9L_3 + {}^{2}C_2H_5 \rightarrow {}^{2}Ir_4CO_8L_3(C_2H_5) + CO \quad (1)$$

$$Ir_4CO_9L_3 + C_2H_4 \rightarrow Ir_4CO_8L_3(C_2H_4) + CO \quad (2)$$

With L = PPh_2(calixarene) corresponding to **1**, the ethylene reaction is least positive at the apical *A1* and *A3* positions. (See Fig. S18 for position labels.) These are the least sterically hindered positions on the apical iridium atom, and on the cluster as a whole. Of the three basal positions, *B1* is the least sterically hindered and the reaction energy for ethylene at *B1* is 4.5 kcal/mol more endothermic than at *A3*. For the reaction of ethyl with the iridium cluster, the two least endothermic apical positions in the ethylene reaction are the same as here (Table S3). The reaction of ethyl bonding with the iridium atom in the *B2* position is the least endothermic of the three basal positions, and this reaction energy is 8.5 kcal/mol more endothermic than that for substitution at the *A1* position.

For the PMe_3 substituted system, the reaction energies of ethylene at the *A1* and *A3* positions are similar due to the presence of two equatorial phosphines and one axial phosphine. Substitution at the *B1* position is less endothermic than at *B2* and *B3* by 3 kcal/mol, but this reaction energy is still 3.2 kcal/mol higher than at *A1*. For the ethyl reaction, substitution at *A3* is less endothermic than substitution at *A1,* and substitution at *B2* is the least endothermic process in the basal plane (Table S4). Substitution at *B2* is still 8.2 kcal/mol more endothermic than at *A3*. Even though there is significantly less steric hindrance in the PMe_3 substituted system than in the calixarene susbstituted system, the preference for apical substitution remains the same.

Additional calculations on the energies of reaction (2) yield energy differences (ΔE_{elec}) of 4.5 kcal/mol for L = PPh_2CH_3, 4.3 kcal/mol for L = $PPh_2(CH_2OCH_3)$, and 9.0 kcal/mol for L = $PPh_2(CH_2OPh)$, consistent with the results for L = PPh_2(calix) and L = PMe_3 with the B3LYP functional (Table S5). Additional results in the Supporting Information show that the preference for apical substitution does not depend on the use of a hybrid versus generalized gradient approximation functional.

Table S3. Calculated reaction energy of ethylene (reaction (2)) with the Ir cluster using ONIOM (B3LYP/LANL2DZ/6-31+G(d,p):UFF) for the Calixarene complex and full DFT (B3LYP/LANL2DZ/6-31+G(d,p)) for the PMe_3 complex. Reaction energies are free energies in kcal/mol

Ethylene Reaction Site	Calixarene Complex	PMe_3 Complex
Apical 1	22.5	23.7
Apical 2	27.0	29.5
Apical 3	20.4	25.4
Basal 1	24.9	26.9
Basal 2	27.6	30.2
Basal 3	28.8	30.2

Table S4. Calculated reaction energy of ethyl (reaction (1)) with the Ir cluster using ONIOM (B3LYP/LANL2DZ/6-31+G(d,p):UFF) for the Calixarene complex and full DFT (B3LYP/LANL2DZ/6-31+G(d,p)) for the PMe_3 complex. Reaction energies are free energies in kcal/mol

Ethyl	Calixarene	PMe_3

Reaction Site	Complex	Complex
Apical 1	6.5	12.4
Apical 2	11.6	17.2
Apical 3	7.4	11.6
Basal 1	23.0	26.5
Basal 2	15.0	19.8
Basal 3	21.4	19.9

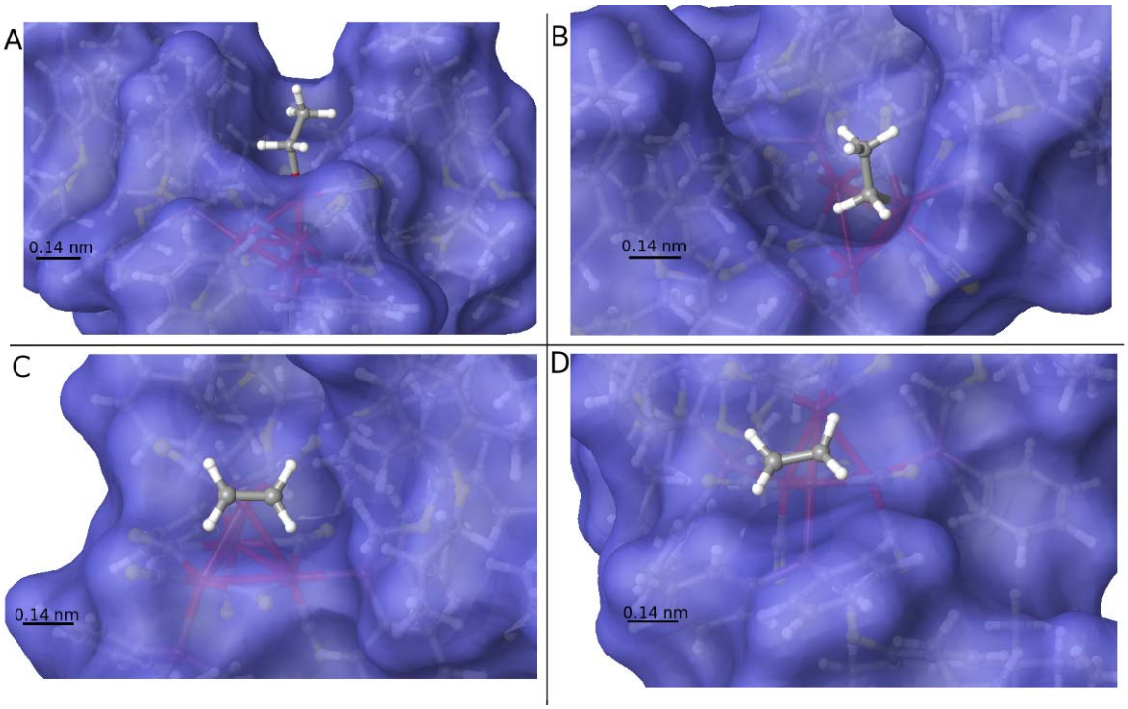


Figure S17. Lowest relative energy structure of : (i) ethyl bound to (A) apical and (B) basal-plane Ir atoms, and (ii) ethylene π-bound to (C) apical and (D) basal-plane Ir atoms, in the calixarene-phosphine Ir_4 cluster.

Additional calculations were done with L = PPh_2CH_3, L = $PPh_2(CH_2OCH_3)$, and L = $PPh_2(CH_2OPh)$ to provide more insight into electronic effects. Following our work on $Ir_x(CO)_y$ clusters, [S12] we optimized the geometries with the SVWN exchange-correlation functional [S13,S14] and the cc-pVDZ-ECP basis set [S15] and ECP on Ir and the DZVP basis set [S16] on the main group elements. Subsequent single point calculations were done with the hybrid B3LYP and pure generalized gradient PW91 [S17-S19] functionals and the same basis set. Prior tests on L = PH_3 show that the electronic ΔE_{elec} and $\Delta H(298)$ energies are essentially the same. There is a slightly larger difference between ΔE_{elec} and $\Delta G(298)$ but it does not affect the conclusions. For L = PPh_2CH_3, $PPh_2(CH_2OCH_3)$ and $PPh_2(CH_2OPh)$, the B3LYP and PW91 functionals (Table S5) show that substitution at the apex is always less endothermic than substitution on the basal iridiums. These results map onto the PMe_3 and PPh_2(calixarane) results given above showing that these electron donating phosphines prefer apical substitution. In all cases substitution at the axial CO in the

basal plane is observed to be thermodynamically preferred over substitution at the equatorial CO position in the basal plane.

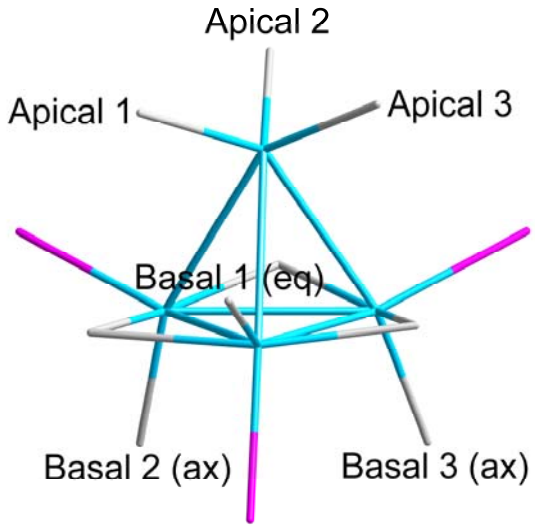


Figure S18. Position assignments for DFT calculations of ethyl- and ethylene binding energies

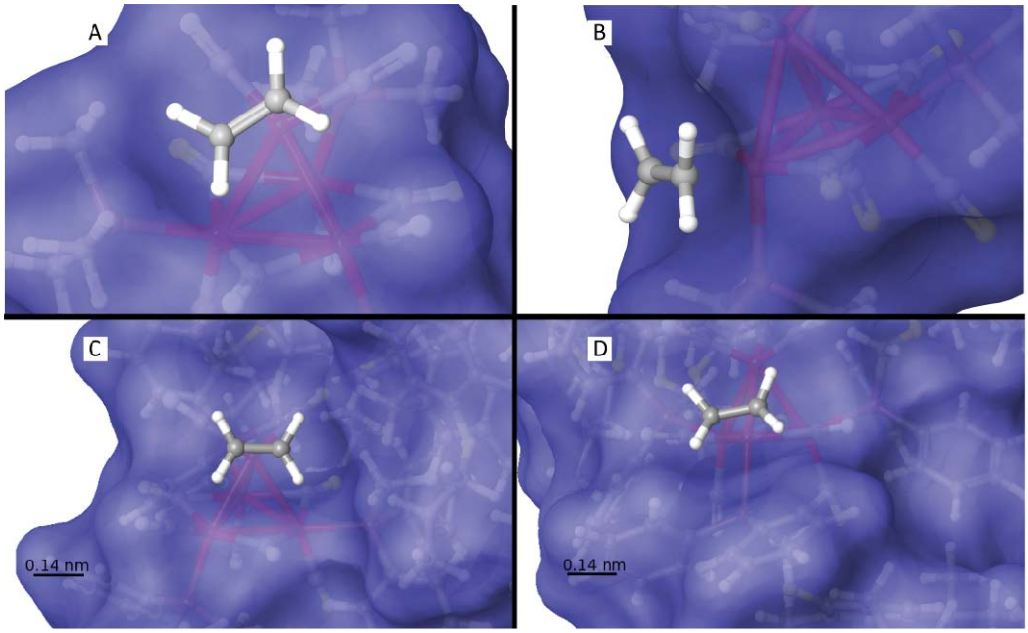


Figure S19. Comparison of ethylene π-bound to a) apical Ir atom and b) basal Ir atom on $Ir_4(CO)_9(PMe_3)_3$ with ethylene bound to c) apical Ir atom and d) basal Ir atom of **1**.

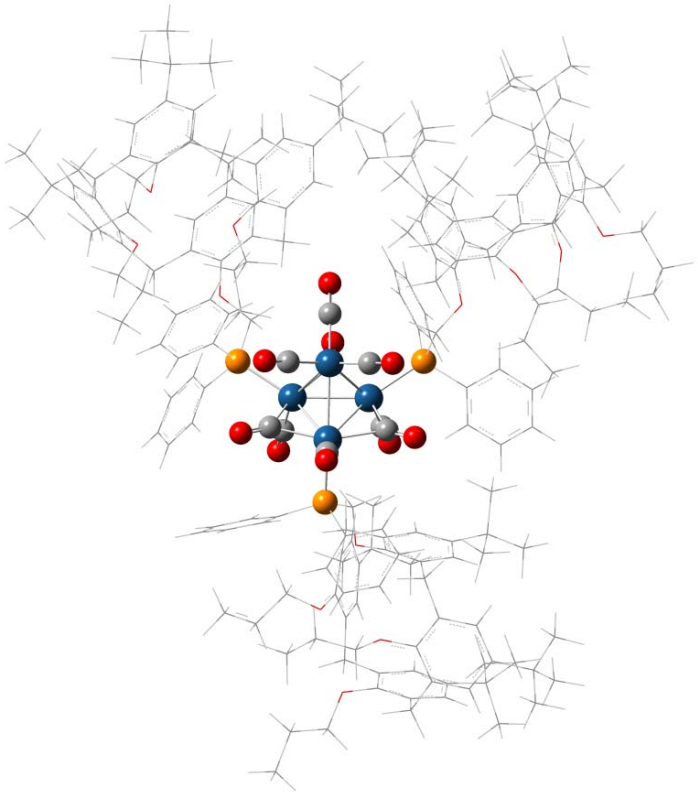


Figure S20. Model system for the ONIOM QM/MM calculations. The visible balls (Ir = blue, P = orange, C = grey, O = red) are the QM region, while the grey wireframe models are the MM region.

Table S5. Reaction Energies (ΔE_{elec}) in kcal/mol for C_2H_4 with L = $PPh_2(CH_2OCH_3)$ and $PPh_2(CH_2OPh)$ with the B3LYP and PW91 DFT Functionals.

Position	Functional	Apical 1	Apical 2	Basal 1 eq	Basal 2 ax
PPh_2CH_3	B3LYP	26.7	27.4	32.4	31.2
$PPh_2(CH_2OCH_3)$	B3LYP	26.1	27.2	31.6	30.4
$PPh_2(CH_2OPh)$	B3LYP	23.0	22.4	36.0	31.4
PPh_2CH_3	PW91	25.7	25.7	30.4	29.8
$PPh_2(CH_2OCH_3)$	PW91	25.6	25.8	29.7	29.4
$PPh_2(CH_2OPh)$	PW91	23.4	22.3	32.4	29.2

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Optimized Cartesian Coordinates in Å

Closed Tetrairidium-Calixarene cluster

0 1

C	0.98350000	-0.87380000	-4.25020000
C	2.15310000	0.07860000	-1.63740000
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H	6.70290000	-5.65510000	5.12020000
H	8.27060000	-4.94690000	5.54320000
C	7.07230000	-3.75160000	4.17780000
C	5.85090000	-3.65530000	3.48140000
C	5.53140000	-2.43480000	2.81640000
C	6.33940000	-1.30540000	3.03950000
H	6.11830000	-0.46850000	2.57620000
C	7.50220000	-1.36390000	3.83100000
C	7.86180000	-2.61040000	4.37740000

H	8.69230000	-2.70840000	4.88810000
C	8.38620000	-0.10740000	3.98250000
C	8.97660000	0.26120000	2.60610000
H	9.61840000	1.16580000	2.68010000
H	8.17630000	0.47210000	1.87010000
H	9.59310000	-0.57590000	2.21220000
C	9.56610000	-0.30870000	4.96470000
H	10.14530000	0.63300000	5.08360000
H	10.27190000	-1.08130000	4.58960000
H	9.19510000	-0.60830000	5.96870000
C	7.53700000	1.07030000	4.51240000
H	8.17040000	1.96970000	4.66990000
H	7.06450000	0.80100000	5.48170000
H	6.73450000	1.35530000	3.80060000
C	3.68010000	-4.58750000	3.70790000
H	3.11790000	-4.86610000	2.79360000
H	3.40800000	-3.55400000	4.02300000
C	3.27480000	-5.51460000	4.85280000
H	3.72000000	-5.14270000	5.80110000
H	3.66660000	-6.53430000	4.67260000
C	1.75760000	-5.58440000	4.99950000
H	1.49680000	-6.25010000	5.84890000
H	1.29970000	-5.99520000	4.07380000
H	1.34200000	-4.57350000	5.19750000
C	4.51410000	-2.34910000	1.68710000
H	4.31480000	-1.28650000	1.42620000
H	3.54060000	-2.72170000	2.01600000
C	-1.53920000	3.65460000	1.22970000
C	-2.83410000	3.57090000	0.86170000
H	-3.13770000	2.86190000	0.25800000
C	-3.77100000	4.50570000	1.33530000
H	-4.71280000	4.43120000	1.06160000
C	-3.38870000	5.49790000	2.16350000
H	-4.05510000	6.14300000	2.49100000
C	-2.10330000	5.61300000	2.54800000
H	-1.83280000	6.33740000	3.15530000
C	-1.14770000	4.69700000	2.08590000
H	-0.21660000	4.77930000	2.37610000
C	0.70140000	1.95970000	2.04910000
C	0.12990000	1.88330000	3.32860000
H	-0.81330000	2.12050000	3.46650000
C	0.89700000	1.45640000	4.41860000
H	0.49420000	1.41060000	5.31390000
C	2.23250000	1.08380000	4.23430000
H	2.76940000	0.78150000	5.00010000
C	2.80160000	1.13420000	2.95900000

H	3.73880000	0.86830000	2.82770000
C	2.03830000	1.56770000	1.87030000
H	2.44610000	1.59070000	0.97850000
C	0.79550000	3.46530000	-0.44490000
H	1.41060000	2.75290000	-1.02980000
H	0.14960000	4.06120000	-1.12100000
C	2.91280000	4.36510000	0.21210000
C	3.71310000	4.52410000	1.36910000
C	5.09340000	4.26620000	1.30090000
H	5.61400000	4.31680000	2.12890000
C	5.71840000	3.90270000	0.09460000
C	4.93240000	3.87120000	-1.06500000
H	5.35780000	3.68110000	-1.92940000
C	3.56770000	4.18990000	-1.04320000
C	7.22330000	3.59070000	-0.00960000
C	7.87620000	4.55610000	-1.02580000
H	7.57140000	5.60150000	-0.81160000
H	7.56660000	4.32530000	-2.06690000
H	8.98500000	4.48900000	-0.98980000
C	7.96570000	3.73610000	1.34130000
H	7.55910000	3.02720000	2.09320000
H	7.87260000	4.77000000	1.73560000
H	9.04860000	3.51410000	1.22490000
C	7.40320000	2.13890000	-0.49740000
H	6.85650000	1.43810000	0.16930000
H	8.47870000	1.85800000	-0.50820000
H	7.00950000	2.00340000	-1.52720000
C	3.11020000	4.80840000	2.73340000
H	2.01820000	4.90730000	2.71110000
H	3.25940000	3.89220000	3.34300000
C	3.79100000	5.99580000	3.40890000
C	3.73690000	7.33410000	2.90830000
C	4.75300000	8.23950000	3.28380000
C	5.69820000	7.88300000	4.25500000
H	6.38100000	8.54250000	4.49830000
C	5.68960000	6.61020000	4.85370000
C	4.72190000	5.68730000	4.41820000
H	4.74670000	4.77280000	4.77430000
C	6.74310000	6.17180000	5.89380000
C	6.03240000	5.71690000	7.18720000
H	5.38680000	4.83150000	7.00910000
H	5.39820000	6.53700000	7.58800000
H	6.77360000	5.43500000	7.96640000
C	7.73090000	7.30190000	6.27290000
H	8.31810000	7.62970000	5.38770000
H	8.45560000	6.95140000	7.03980000

H	7.18850000	8.17470000	6.69670000
C	7.56840000	4.99820000	5.32140000
H	8.05340000	5.29580000	4.36650000
H	6.93180000	4.11070000	5.12500000
H	8.36200000	4.68780000	6.03530000
C	1.45610000	7.34510000	2.19790000
H	1.24460000	6.89970000	3.19640000
H	1.25410000	6.61100000	1.39880000
C	0.49890000	8.52030000	1.99820000
H	0.77030000	9.07060000	1.07490000
H	-0.53450000	8.13260000	1.87260000
C	0.52410000	9.48240000	3.18290000
H	-0.18000000	10.31990000	2.99460000
H	1.54150000	9.90150000	3.32320000
H	0.21210000	8.95910000	4.11170000
C	4.84090000	9.60660000	2.63870000
H	3.83050000	10.05980000	2.60070000
H	5.45780000	10.30100000	3.25060000
C	5.46570000	9.47680000	1.26970000
C	4.71020000	9.63250000	0.08990000
C	5.28410000	9.29800000	-1.15220000
C	6.64750000	8.95690000	-1.21550000
H	7.03550000	8.77490000	-2.09670000
C	7.45490000	8.92550000	-0.05740000
C	6.82990000	9.16290000	1.18130000
H	7.35600000	9.12610000	2.00900000
C	8.98540000	8.72060000	-0.11370000
C	9.67420000	10.05030000	0.25450000
H	9.36890000	10.85330000	-0.45100000
H	10.78030000	9.94710000	0.21010000
H	9.40210000	10.37090000	1.28290000
C	9.48510000	8.29410000	-1.51610000
H	9.29700000	9.09100000	-2.26760000
H	8.98470000	7.35880000	-1.84580000
H	10.58110000	8.10810000	-1.50610000
C	9.42800000	7.63340000	0.89390000
H	8.86390000	6.69710000	0.72900000
H	9.26990000	7.95230000	1.94500000
H	10.51130000	7.40940000	0.78530000
C	3.39200000	11.57800000	0.20120000
H	3.91030000	12.00910000	-0.68530000
H	3.92590000	11.92830000	1.11190000
C	1.95340000	12.09440000	0.26500000
H	1.96200000	13.14080000	0.63970000
H	1.36530000	11.48260000	0.98120000
C	1.27750000	12.08090000	-1.10380000

H	0.22820000	12.42950000	-1.00260000
H	1.27000000	11.06010000	-1.53110000
H	1.81060000	12.76050000	-1.80210000
C	4.47910000	9.34940000	-2.43270000
H	4.97550000	10.06990000	-3.11900000
H	3.46340000	9.75840000	-2.27710000
C	4.39710000	7.97670000	-3.07080000
C	3.56900000	6.95840000	-2.54370000
C	3.66500000	5.64950000	-3.05100000
C	4.51160000	5.38260000	-4.13530000
H	4.56750000	4.46310000	-4.47470000
C	5.31300000	6.38870000	-4.70910000
C	5.23820000	7.68600000	-4.15850000
H	5.80530000	8.40480000	-4.50730000
C	6.27150000	6.02860000	-5.86420000
C	7.06990000	7.24480000	-6.39380000
H	7.73220000	6.94570000	-7.23520000
H	7.71770000	7.67190000	-5.59760000
H	6.38370000	8.03400000	-6.77060000
C	5.46230000	5.44930000	-7.04510000
H	6.12770000	5.22350000	-7.90650000
H	4.69230000	6.17790000	-7.37950000
H	4.95080000	4.50440000	-6.76580000
C	7.28970000	4.97620000	-5.37320000
H	8.01570000	4.72520000	-6.17660000
H	6.78850000	4.03310000	-5.06970000
H	7.85600000	5.36590000	-4.49950000
C	1.52950000	7.97500000	-1.82430000
H	1.56450000	8.36650000	-2.86780000
H	1.48580000	8.83850000	-1.13640000
C	0.26110000	7.13650000	-1.65690000
H	0.28330000	6.60220000	-0.68630000
H	0.20490000	6.38530000	-2.47210000
C	-0.99130000	8.00600000	-1.71030000
H	-1.89200000	7.36570000	-1.60050000
H	-1.04860000	8.53980000	-2.68270000
H	-0.98270000	8.74840000	-0.88410000
C	2.92590000	4.51100000	-2.38060000
H	2.94860000	3.59560000	-3.01080000
H	1.87450000	4.81810000	-2.29350000
C	-5.61250000	-0.07000000	-3.74910000
C	-5.54420000	1.33080000	-3.76560000
H	-4.89170000	1.79940000	-3.20340000
C	-6.41660000	2.07410000	-4.56670000
H	-6.36690000	3.05580000	-4.56760000
C	-7.36180000	1.42180000	-5.36230000

H	-7.97550000	1.94380000	-5.92520000
C	-7.43660000	0.02630000	-5.35360000
H	-8.10490000	-0.43120000	-5.91020000
C	-6.57230000	-0.71860000	-4.54330000
H	-6.65580000	-1.69530000	-4.53240000
C	-4.71320000	-2.77790000	-2.98710000
C	-4.49050000	-3.30300000	-4.26800000
H	-4.26120000	-2.70850000	-5.01650000
C	-4.57430000	-4.68690000	-4.47680000
H	-4.41920000	-5.05190000	-5.37650000
C	-4.84530000	-5.51940000	-3.45240000
H	-4.88670000	-6.48870000	-3.61450000
C	-5.05000000	-5.04720000	-2.20720000
H	-5.22790000	-5.67280000	-1.47050000
C	-5.00050000	-3.67100000	-1.94700000
H	-5.13490000	-3.35080000	-1.03250000
C	-5.00190000	-0.60720000	-0.97920000
H	-4.42470000	-1.22750000	-0.26640000
H	-4.74190000	0.46290000	-0.81520000
C	-6.87000000	-0.12440000	0.33350000
C	-6.59490000	-0.60030000	1.63410000
C	-6.71210000	0.27580000	2.72410000
H	-6.44770000	-0.04130000	3.61410000
C	-7.19010000	1.58910000	2.57210000
C	-7.58620000	1.99870000	1.28300000
H	-7.95010000	2.89660000	1.13560000
C	-7.44040000	1.15450000	0.16960000
C	-7.25580000	2.51720000	3.80250000
C	-5.82400000	2.77460000	4.31780000
H	-5.20420000	3.23950000	3.52230000
H	-5.33010000	1.83040000	4.63160000
H	-5.83800000	3.45720000	5.19500000
C	-8.08300000	1.84080000	4.91920000
H	-9.05150000	1.48090000	4.51780000
H	-8.28310000	2.54630000	5.75440000
H	-7.54800000	0.96880000	5.34880000
C	-7.90260000	3.88890000	3.49120000
H	-8.93750000	3.76060000	3.10850000
H	-7.30370000	4.44840000	2.74000000
H	-7.95550000	4.51770000	4.40630000
C	-6.17580000	-2.03090000	1.89690000
H	-6.03690000	-2.59150000	0.96220000
H	-5.17050000	-2.01450000	2.37190000
C	-7.19000000	-2.70300000	2.81300000
C	-8.50170000	-3.03330000	2.37110000
C	-9.53800000	-3.13620000	3.31860000

C	-9.23790000	-3.11650000	4.68700000
H	-9.96960000	-3.22920000	5.33180000
C	-7.92170000	-2.93550000	5.15070000
C	-6.91020000	-2.71810000	4.19170000
H	-5.99890000	-2.50070000	4.47880000
C	-7.64730000	-2.92390000	6.67010000
C	-8.47240000	-1.80130000	7.33800000
H	-9.56370000	-1.97350000	7.22930000
H	-8.22870000	-0.81870000	6.88190000
H	-8.25260000	-1.74470000	8.42620000
C	-8.05550000	-4.28560000	7.27220000
H	-9.14180000	-4.47750000	7.14540000
H	-7.83610000	-4.31720000	8.36160000
H	-7.49590000	-5.10950000	6.77860000
C	-6.15800000	-2.68260000	7.01690000
H	-5.51520000	-3.47410000	6.57420000
H	-6.00130000	-2.70040000	8.11750000
H	-5.82170000	-1.68880000	6.64910000
C	-7.98320000	-4.12520000	0.33810000
H	-7.14410000	-4.55170000	0.93680000
H	-7.56510000	-3.56530000	-0.52330000
C	-8.84680000	-5.29650000	-0.15950000
H	-9.20880000	-5.87020000	0.72420000
H	-9.74070000	-4.89210000	-0.67620000
C	-8.20030000	-6.09520000	-0.97060000
H	-8.86300000	-6.92910000	-1.29340000
H	-7.31450000	-6.54450000	-0.46830000
H	-7.87390000	-5.55350000	-1.88680000
C	-10.97560000	-3.31000000	2.87660000
H	-11.02330000	-4.04570000	2.04650000
H	-11.58860000	-3.74880000	3.69430000
C	-11.57140000	-1.97250000	2.49500000
C	-11.91960000	-1.67120000	1.16240000
C	-12.40590000	-0.38700000	0.84120000
C	-12.65960000	0.53240000	1.86970000
H	-13.04680000	1.40360000	1.63560000
C	-12.35980000	0.24180000	3.21320000
C	-11.79320000	-1.01770000	3.50270000
H	-11.56010000	-1.25840000	4.42370000
C	-12.67950000	1.28600000	4.30450000
C	-12.03420000	2.64430000	3.94190000
H	-12.50940000	3.10030000	3.04850000
H	-10.95530000	2.51550000	3.72670000
H	-12.14270000	3.37240000	4.77470000
C	-14.20900000	1.46330000	4.39600000
H	-14.63050000	1.83000000	3.43580000

H	-14.47340000	2.19950000	5.18590000
H	-14.69680000	0.49510000	4.64160000
C	-12.16190000	0.87430000	5.70470000
H	-12.37740000	1.66630000	6.45440000
H	-11.06290000	0.71310000	5.68870000
H	-12.65990000	-0.05500000	6.05620000
C	-12.97870000	-3.34700000	-0.10670000
H	-13.78410000	-2.63660000	-0.39920000
H	-13.30390000	-3.90050000	0.80280000
C	-12.75020000	-4.33860000	-1.24470000
H	-12.02810000	-5.11480000	-0.91730000
H	-12.32700000	-3.80450000	-2.12280000
C	-14.05080000	-5.02240000	-1.65490000
H	-13.84790000	-5.74540000	-2.47280000
H	-14.78380000	-4.27130000	-2.01920000
H	-14.48560000	-5.57260000	-0.79340000
C	-12.62870000	0.05010000	-0.59010000
H	-12.52140000	-0.78610000	-1.30560000
H	-13.67890000	0.40100000	-0.69260000
C	-11.65500000	1.15600000	-0.93890000
C	-10.28860000	0.88060000	-1.15100000
C	-9.36020000	1.93860000	-1.19070000
C	-9.81570000	3.26510000	-1.15220000
H	-9.14940000	3.98260000	-1.18760000
C	-11.18830000	3.56580000	-1.01600000
C	-12.09170000	2.48880000	-0.90570000
H	-13.04530000	2.66860000	-0.75670000
C	-11.71630000	5.01240000	-0.91560000
C	-12.37550000	5.22050000	0.46560000
H	-12.72820000	6.26840000	0.58030000
H	-11.64670000	5.00580000	1.27730000
H	-13.25420000	4.55590000	0.60340000
C	-12.76070000	5.25860000	-2.02630000
H	-12.31330000	5.06810000	-3.02580000
H	-13.12450000	6.30870000	-2.00020000
H	-13.64580000	4.59880000	-1.90860000
C	-10.60400000	6.07780000	-1.07280000
H	-10.09610000	5.97610000	-2.05630000
H	-9.85060000	5.98840000	-0.26030000
H	-11.02970000	7.10340000	-1.01840000
C	-9.92050000	-0.89480000	-2.56470000
H	-9.33560000	-0.25710000	-3.26340000
H	-10.97130000	-0.93150000	-2.92500000
C	-9.33160000	-2.30020000	-2.57230000
H	-8.24020000	-2.24030000	-2.37570000
H	-9.80950000	-2.89040000	-1.76690000

C	-9.56400000	-3.00770000	-3.90290000
H	-9.08980000	-4.01130000	-3.87520000
H	-9.11870000	-2.42680000	-4.73620000
H	-10.65200000	-3.13400000	-4.08700000
C	-7.87400000	1.65680000	-1.18970000
H	-7.29290000	2.57410000	-1.42890000
H	-7.65130000	0.92570000	-1.99000000
O	1.26370000	-1.38880000	-5.24380000
O	3.17020000	0.07740000	-1.08450000
O	0.38920000	2.89390000	-3.91220000
O	-2.81040000	-3.49020000	0.41170000
O	0.69070000	-1.07920000	1.35680000
O	-3.23620000	0.21330000	1.78780000
O	-2.59860000	2.64900000	-2.31270000
O	-2.51370000	0.47090000	-5.86820000
O	-1.38240000	-3.18190000	-4.06530000
O	3.07390000	-4.55170000	0.16290000
O	5.23070000	-7.45240000	0.71250000
O	6.63260000	-7.65570000	3.62400000
O	5.08270000	-4.74420000	3.45310000
O	1.58620000	4.33850000	0.37760000
O	2.80630000	7.80110000	2.07290000
O	3.40720000	10.14710000	0.14410000
O	2.68850000	7.20610000	-1.47860000
O	-6.40600000	-0.81780000	-0.79610000
O	-8.81880000	-3.23540000	1.09420000
O	-11.76580000	-2.63830000	0.16080000
O	-9.85890000	-0.36920000	-1.23280000
P	0.81290000	-3.83530000	-1.18680000
P	-0.30970000	2.44920000	0.60910000
P	-4.45670000	-0.99710000	-2.68550000
Ir	0.52180000	0.08810000	-2.64240000
Ir	-0.73270000	-2.02190000	-1.25420000
Ir	-1.22090000	0.54740000	-0.47280000
Ir	-2.17600000	-0.37050000	-2.98460000

Π-bound Ethylene at the Apical 3 on the Tetrairidium-Calixarene complex

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C	-1.81320000	-3.24440000	-0.34200000
C	0.11270000	-1.03270000	0.07410000
C	-2.44110000	0.12220000	0.54300000
C	-2.18020000	1.06700000	-2.60350000
C	-2.59350000	-0.69790000	-5.07040000
C	-1.41350000	-2.90370000	-3.36170000
C	0.28730000	-5.61810000	-0.68860000
C	0.62210000	-6.22790000	0.53730000

H	1.38750000	-5.81380000	1.17270000
C	-0.02750000	-7.32530000	0.96380000
H	0.23250000	-7.76660000	1.91670000
C	-1.05310000	-7.89390000	0.20050000
H	-1.56900000	-8.77620000	0.55660000
C	-1.42250000	-7.30990000	-1.01200000
H	-2.22740000	-7.73280000	-1.59940000
C	-0.75820000	-6.16400000	-1.45210000
H	-1.06720000	-5.69900000	-2.37620000
C	2.06740000	-4.36520000	-2.70800000
C	1.90900000	-5.53160000	-3.47610000
H	1.18800000	-6.28640000	-3.20870000
C	2.69350000	-5.73920000	-4.61570000
H	2.56250000	-6.63740000	-5.20520000
C	3.65470000	-4.79650000	-4.98800000
H	4.26700000	-4.96360000	-5.86460000
C	3.83440000	-3.64500000	-4.21950000
H	4.58700000	-2.91910000	-4.49900000
C	3.04040000	-3.42750000	-3.08980000
H	3.19610000	-2.53060000	-2.50950000
C	2.25470000	-3.54980000	0.07440000
H	2.60060000	-2.52850000	-0.19180000
H	1.71480000	-3.49400000	1.04090000
C	4.61720000	-3.98180000	-0.10910000
C	5.37280000	-4.64710000	-1.09440000
C	6.49410000	-4.01660000	-1.64930000
H	6.99410000	-4.49330000	-2.48050000
C	6.98440000	-2.80180000	-1.14650000
C	6.31390000	-2.22950000	-0.04720000
H	6.66770000	-1.31060000	0.39400000
C	5.15420000	-2.81090000	0.49670000
C	8.22300000	-2.15900000	-1.80350000
C	7.85520000	-1.71210000	-3.23350000
H	7.53420000	-2.57410000	-3.85640000
H	8.72720000	-1.23710000	-3.73320000
H	7.02180000	-0.97670000	-3.20690000
C	9.37490000	-3.19050000	-1.87130000
H	9.18340000	-3.96950000	-2.63800000
H	9.49430000	-3.70110000	-0.89420000
H	10.33760000	-2.70440000	-2.13990000
C	8.73990000	-0.91890000	-1.03500000
H	9.65440000	-0.50730000	-1.51450000
H	8.99430000	-1.18040000	0.01410000
H	7.97950000	-0.11030000	-1.03530000
C	5.00860000	-6.03120000	-1.58720000
H	4.09620000	-6.42380000	-1.09670000

H	4.77410000	-5.96700000	-2.66790000
C	6.17480000	-6.97310000	-1.36320000
C	6.52400000	-7.39920000	-0.06670000
C	7.77380000	-8.01060000	0.15700000
C	8.60540000	-8.30770000	-0.93390000
H	9.55150000	-8.78430000	-0.72680000
C	8.23720000	-7.96600000	-2.25370000
C	7.01390000	-7.29110000	-2.44160000
H	6.73020000	-6.95840000	-3.43110000
C	9.14390000	-8.24490000	-3.47120000
C	8.37240000	-9.09230000	-4.50690000
H	7.49060000	-8.54960000	-4.90660000
H	8.01960000	-10.03960000	-4.04450000
H	9.02250000	-9.34670000	-5.37200000
C	9.56510000	-6.90500000	-4.11350000
H	8.68910000	-6.33770000	-4.49170000
H	10.24720000	-7.07790000	-4.97410000
H	10.09540000	-6.27160000	-3.36990000
C	10.43520000	-9.01660000	-3.10580000
H	10.19180000	-9.99580000	-2.63960000
H	11.06950000	-8.42450000	-2.41100000
H	11.04340000	-9.21980000	-4.01410000
C	4.72670000	-8.25900000	1.06670000
H	5.24020000	-9.23190000	1.23920000
H	4.11230000	-8.34770000	0.14330000
C	3.80730000	-7.96620000	2.24440000
H	4.42150000	-7.82410000	3.15430000
H	3.24590000	-7.03100000	2.04760000
C	2.82400000	-9.10730000	2.48250000
H	2.15280000	-8.84700000	3.32780000
H	3.36900000	-10.04060000	2.73740000
H	2.20910000	-9.28300000	1.57470000
C	8.25500000	-8.30330000	1.56160000
H	9.11130000	-9.01230000	1.54760000
H	7.45300000	-8.81970000	2.12490000
C	8.70340000	-7.02820000	2.24250000
C	8.01800000	-6.50860000	3.35930000
C	8.41900000	-5.27420000	3.91030000
C	9.59130000	-4.66090000	3.44480000
H	9.92740000	-3.75810000	3.93420000
C	10.32410000	-5.18430000	2.36420000
C	9.84290000	-6.36410000	1.75610000
H	10.35660000	-6.80500000	0.91520000
C	11.62200000	-4.47780000	1.91570000
C	11.35280000	-2.97510000	1.66010000
H	12.23710000	-2.48380000	1.19950000

H	11.13530000	-2.42620000	2.59970000
H	10.48830000	-2.84550000	0.98110000
C	12.67730000	-4.61630000	3.03210000
H	13.63130000	-4.12910000	2.73470000
H	12.88150000	-5.68890000	3.24090000
H	12.33180000	-4.14000000	3.97430000
C	12.21840000	-5.07610000	0.61830000
H	13.12390000	-4.51350000	0.30310000
H	11.48330000	-5.02740000	-0.21330000
H	12.52900000	-6.13210000	0.77120000
C	7.35370000	-7.99430000	5.06010000
H	7.69250000	-7.31710000	5.87420000
H	8.20090000	-8.66970000	4.80100000
C	6.17710000	-8.82210000	5.57850000
H	6.40000000	-9.16200000	6.61300000
H	5.26260000	-8.19260000	5.61550000
C	5.92280000	-10.05150000	4.70980000
H	5.01950000	-10.58430000	5.07420000
H	6.78950000	-10.74410000	4.76240000
H	5.76130000	-9.75990000	3.65350000
C	7.59970000	-4.55920000	4.96160000
H	6.76690000	-5.18300000	5.34720000
H	8.24890000	-4.34580000	5.83880000
C	7.04160000	-3.27760000	4.37760000
C	5.86450000	-3.29450000	3.60340000
C	5.49370000	-2.11870000	2.88670000
C	6.19910000	-0.92600000	3.12360000
H	5.91780000	-0.04090000	2.56920000
C	7.31060000	-0.87320000	3.98620000
C	7.72440000	-2.07300000	4.59600000
H	8.60180000	-2.10240000	5.22380000
C	8.08740000	0.45090000	4.14740000
C	8.72210000	0.83070000	2.79330000
H	9.29600000	1.77890000	2.87730000
H	7.95020000	0.97040000	2.01170000
H	9.41420000	0.03030000	2.45200000
C	9.22600000	0.36780000	5.19320000
H	9.72320000	1.35500000	5.31380000
H	10.00930000	-0.35420000	4.87570000
H	8.82740000	0.06670000	6.18610000
C	7.12470000	1.57200000	4.60070000
H	7.67950000	2.52070000	4.76510000
H	6.62380000	1.29040000	5.55200000
H	6.34130000	1.77920000	3.84280000
C	3.76600000	-4.39070000	3.74180000
H	3.27230000	-4.73120000	2.80960000

H	3.39850000	-3.37560000	4.01770000
C	3.37960000	-5.32360000	4.88870000
H	3.74110000	-4.89430000	5.84820000
H	3.86490000	-6.30990000	4.75590000
C	1.86790000	-5.51950000	4.95970000
H	1.61920000	-6.18430000	5.81340000
H	1.49600000	-5.99040000	4.02420000
H	1.35870000	-4.54330000	5.10710000
C	4.53210000	-2.13540000	1.70700000
H	4.26750000	-1.09800000	1.40580000
H	3.57380000	-2.56980000	2.00100000
C	-1.84980000	3.42010000	0.61760000
C	-3.08980000	3.24020000	0.11710000
H	-3.30100000	2.43490000	-0.56750000
C	-4.13610000	4.10560000	0.47790000
H	-5.12630000	3.94830000	0.06890000
C	-3.91680000	5.12520000	1.32960000
H	-4.73290000	5.78280000	1.60100000
C	-2.69480000	5.33030000	1.85270000
H	-2.53260000	6.14420000	2.54750000
C	-1.63110000	4.48750000	1.50390000
H	-0.66040000	4.65230000	1.93800000
C	0.43110000	1.92880000	1.66910000
C	-0.24610000	1.82740000	2.89460000
H	-1.31150000	2.00740000	2.95350000
C	0.44880000	1.47550000	4.05600000
H	-0.07690000	1.40580000	4.99950000
C	1.81790000	1.20010000	3.99870000
H	2.35340000	0.92390000	4.89770000
C	2.49350000	1.27150000	2.77850000
H	3.55200000	1.05150000	2.73250000
C	1.80360000	1.63200000	1.61760000
H	2.33880000	1.66310000	0.67860000
C	0.64430000	3.41900000	-0.82060000
H	1.36600000	2.76820000	-1.35610000
H	0.01290000	3.97590000	-1.54110000
C	2.61410000	4.50940000	0.00460000
C	3.31540000	4.71670000	1.21790000
C	4.71430000	4.57500000	1.24490000
H	5.20830000	4.65330000	2.20070000
C	5.45050000	4.28670000	0.08060000
C	4.75340000	4.23300000	-1.13360000
H	5.29880000	4.08570000	-2.05620000
C	3.36910000	4.43710000	-1.20280000
C	6.97580000	4.06620000	0.08000000
C	7.64410000	5.08250000	-0.87590000

H	7.25270000	6.10320000	-0.68660000
H	7.44270000	4.84020000	-1.94030000
H	8.74800000	5.09130000	-0.74700000
C	7.61210000	4.23340000	1.48120000
H	7.19990000	3.48800000	2.19330000
H	7.43100000	5.25350000	1.88060000
H	8.71190000	4.07780000	1.43840000
C	7.27480000	2.63340000	-0.40840000
H	6.72600000	1.89270000	0.21190000
H	8.36290000	2.41360000	-0.34750000
H	6.96120000	2.48910000	-1.46400000
C	2.59740000	4.91850000	2.54010000
H	1.50600000	4.91950000	2.43970000
H	2.78550000	4.00700000	3.14420000
C	3.11380000	6.14710000	3.28460000
C	2.96780000	7.48780000	2.81040000
C	3.84890000	8.47850000	3.29430000
C	4.73970000	8.18910000	4.33620000
H	5.38310000	8.98450000	4.68060000
C	4.81190000	6.90310000	4.90280000
C	3.98320000	5.90240000	4.36350000
H	4.07520000	4.89090000	4.73510000
C	5.81080000	6.53890000	6.02230000
C	5.04120000	5.98020000	7.23930000
H	4.50590000	5.04030000	6.99030000
H	4.29550000	6.72230000	7.59810000
H	5.73730000	5.75180000	8.07550000
C	6.64620000	7.74670000	6.51190000
H	7.27460000	8.15450000	5.69050000
H	7.33250000	7.44460000	7.33270000
H	5.98660000	8.55000000	6.90570000
C	6.79610000	5.46910000	5.50120000
H	7.32330000	5.83750000	4.59440000
H	6.27350000	4.52640000	5.23890000
H	7.55710000	5.22280000	6.27310000
C	0.76210000	7.30990000	1.91430000
H	0.51640000	6.81620000	2.88160000
H	0.68820000	6.58550000	1.08470000
C	-0.27630000	8.40580000	1.67160000
H	0.03010000	9.02740000	0.80680000
H	-1.25250000	7.93810000	1.42380000
C	-0.45460000	9.30140000	2.89460000
H	-1.20660000	10.08720000	2.67170000
H	0.50340000	9.79390000	3.15980000
H	-0.81170000	8.70480000	3.76080000
C	3.84690000	9.86800000	2.69230000

H	2.80160000	10.22340000	2.59670000
H	4.35230000	10.59930000	3.36050000
C	4.56770000	9.84060000	1.36630000
C	3.87920000	9.96110000	0.14250000
C	4.56090000	9.71470000	-1.06470000
C	5.95060000	9.49790000	-1.04370000
H	6.44940000	9.36420000	-1.99110000
C	6.68000000	9.49890000	0.16580000
C	5.95670000	9.65050000	1.36350000
H	6.47220000	9.63680000	2.31380000
C	8.22120000	9.40330000	0.21360000
C	8.78730000	10.76190000	0.67430000
H	8.47740000	11.56810000	-0.02540000
H	9.89820000	10.73500000	0.70800000
H	8.42180000	11.02560000	1.68980000
C	8.84880000	9.06550000	-1.16110000
H	8.66040000	9.87630000	-1.89740000
H	8.44240000	8.11010000	-1.55660000
H	9.95180000	8.95530000	-1.07640000
C	8.66650000	8.30980000	1.21360000
H	8.15710000	7.35310000	0.99470000
H	8.44020000	8.58850000	2.26330000
H	9.76370000	8.14140000	1.15740000
C	2.38540000	11.77660000	0.20900000
H	2.91300000	12.27640000	-0.63490000
H	2.83090000	12.14770000	1.15830000
C	0.90510000	12.16150000	0.19710000
H	0.80040000	13.20220000	0.57350000
H	0.33760000	11.49490000	0.88010000
C	0.30640000	12.09600000	-1.20550000
H	-0.77150000	12.35810000	-1.16110000
H	0.40390000	11.07830000	-1.62880000
H	0.81910000	12.81740000	-1.87670000
C	3.83880000	9.72400000	-2.39430000
H	4.29870000	10.51450000	-3.02660000
H	2.77730000	10.01930000	-2.29660000
C	3.94370000	8.37120000	-3.06990000
C	3.19630000	7.25590000	-2.62470000
C	3.46860000	5.98050000	-3.15080000
C	4.41300000	5.83730000	-4.17640000
H	4.60650000	4.84670000	-4.56530000
C	5.13800000	6.93850000	-4.67130000
C	4.88240000	8.20450000	-4.10210000
H	5.43670000	9.07440000	-4.42000000
C	6.20820000	6.71340000	-5.76070000
C	6.91030000	8.01930000	-6.20590000

H	7.65740000	7.81320000	-7.00310000
H	7.45450000	8.48730000	-5.35700000
H	6.17430000	8.74370000	-6.61710000
C	5.55030000	6.08830000	-7.01060000
H	6.29470000	5.96030000	-7.82620000
H	4.73220000	6.74190000	-7.38360000
H	5.12470000	5.08670000	-6.79300000
C	7.29580000	5.75920000	-5.21940000
H	8.10230000	5.61400000	-5.97060000
H	6.88090000	4.75790000	-4.97990000
H	7.75030000	6.17730000	-4.29490000
C	1.01120000	8.03090000	-2.05150000
H	1.08300000	8.44760000	-3.08330000
H	0.82620000	8.87050000	-1.35810000
C	-0.17060000	7.06090000	-1.99530000
H	-0.15980000	6.50090000	-1.03920000
H	-0.09090000	6.33350000	-2.83000000
C	-1.50110000	7.79710000	-2.11710000
H	-2.33460000	7.06380000	-2.08660000
H	-1.54780000	8.35190000	-3.07830000
H	-1.62710000	8.51040000	-1.27500000
C	2.80160000	4.75020000	-2.57330000
H	2.97940000	3.87450000	-3.22770000
H	1.71870000	4.93740000	-2.56330000
C	-5.72430000	-0.75020000	-3.81350000
C	-5.65590000	0.64540000	-3.93400000
H	-4.91120000	1.20490000	-3.38750000
C	-6.56470000	1.33270000	-4.74280000
H	-6.51010000	2.41060000	-4.82250000
C	-7.54380000	0.62910000	-5.44640000
H	-8.24590000	1.16070000	-6.07550000
C	-7.61890000	-0.76100000	-5.33490000
H	-8.37850000	-1.30280000	-5.88240000
C	-6.72170000	-1.45040000	-4.51190000
H	-6.82050000	-2.52180000	-4.42180000
C	-4.74780000	-3.39730000	-2.92890000
C	-4.56180000	-4.00270000	-4.17970000
H	-4.34860000	-3.40250000	-5.05540000
C	-4.63240000	-5.39760000	-4.29430000
H	-4.49070000	-5.86230000	-5.26170000
C	-4.85510000	-6.16380000	-3.20970000
H	-4.89170000	-7.24060000	-3.31690000
C	-5.02210000	-5.61450000	-1.99210000
H	-5.17870000	-6.25200000	-1.13200000
C	-4.98150000	-4.22450000	-1.82280000
H	-5.09320000	-3.81640000	-0.83470000

C	-4.92700000	-1.08210000	-1.05520000
H	-4.31060000	-1.65960000	-0.33890000
H	-4.63910000	-0.00860000	-1.00020000
C	-6.65600000	-0.46900000	0.37740000
C	-6.31600000	-0.91000000	1.67490000
C	-6.27180000	0.01760000	2.72630000
H	-5.91680000	-0.31420000	3.69130000
C	-6.64820000	1.36010000	2.54860000
C	-7.11660000	1.74640000	1.27630000
H	-7.44340000	2.75780000	1.08800000
C	-7.12890000	0.84750000	0.19700000
C	-6.50770000	2.34630000	3.72640000
C	-5.01130000	2.50590000	4.07090000
H	-4.44520000	2.86620000	3.18570000
H	-4.56440000	1.54140000	4.39290000
H	-4.87260000	3.23620000	4.89720000
C	-7.25820000	1.79800000	4.96240000
H	-8.28830000	1.49500000	4.68690000
H	-7.31630000	2.56150000	5.76810000
H	-6.74580000	0.91330000	5.39280000
C	-7.07640000	3.75090000	3.41140000
H	-8.15230000	3.69100000	3.14250000
H	-6.51950000	4.22800000	2.57770000
H	-6.98420000	4.42190000	4.29290000
C	-5.97580000	-2.35310000	1.97260000
H	-5.93410000	-2.95370000	1.05650000
H	-4.94220000	-2.38820000	2.38110000
C	-6.97170000	-2.91990000	2.97490000
C	-8.32950000	-3.17090000	2.62860000
C	-9.30740000	-3.14210000	3.64140000
C	-8.91900000	-3.08840000	4.98620000
H	-9.68790000	-3.11580000	5.74640000
C	-7.56610000	-2.99440000	5.36110000
C	-6.60500000	-2.90000000	4.33260000
H	-5.56580000	-2.72670000	4.56750000
C	-7.19760000	-2.93300000	6.85910000
C	-7.88240000	-1.71130000	7.51210000
H	-8.98870000	-1.79430000	7.48260000
H	-7.59050000	-0.77770000	6.98600000
H	-7.58640000	-1.61720000	8.57950000
C	-7.67830000	-4.22370000	7.55730000
H	-8.78230000	-4.32780000	7.50900000
H	-7.39170000	-4.22160000	8.63150000
H	-7.22250000	-5.11580000	7.07560000
C	-5.67520000	-2.80470000	7.10790000
H	-5.12810000	-3.66680000	6.66840000

H	-5.45360000	-2.78910000	8.19730000
H	-5.28110000	-1.85860000	6.67720000
C	-7.99670000	-4.37210000	0.61370000
H	-7.15690000	-4.83680000	1.18000000
H	-7.59440000	-3.86820000	-0.28820000
C	-8.93600000	-5.50160000	0.19020000
H	-9.29040000	-6.04200000	1.09460000
H	-9.82060000	-5.08150000	-0.32580000
C	-8.24680000	-6.48710000	-0.74630000
H	-8.96060000	-7.28810000	-1.03220000
H	-7.37580000	-6.95380000	-0.24000000
H	-7.91020000	-5.96870000	-1.66920000
C	-10.78040000	-3.20710000	3.29970000
H	-10.94340000	-3.95760000	2.49810000
H	-11.37030000	-3.57360000	4.16820000
C	-11.29200000	-1.83510000	2.91680000
C	-11.71470000	-1.54340000	1.60410000
C	-12.12120000	-0.23400000	1.27550000
C	-12.21470000	0.73370000	2.28560000
H	-12.58190000	1.71620000	2.02240000
C	-11.83290000	0.46000000	3.61180000
C	-11.35680000	-0.83650000	3.90380000
H	-11.04590000	-1.10110000	4.90280000
C	-11.96270000	1.56630000	4.68050000
C	-11.21330000	2.83750000	4.21660000
H	-11.71170000	3.31790000	3.34930000
H	-10.17610000	2.58680000	3.91880000
H	-11.17350000	3.59640000	5.02770000
C	-13.45520000	1.90320000	4.87830000
H	-13.91230000	2.28200000	3.93960000
H	-13.58200000	2.68680000	5.65660000
H	-14.01700000	0.99850000	5.19690000
C	-11.38240000	1.15240000	6.05500000
H	-11.46070000	1.98740000	6.78480000
H	-10.30850000	0.88180000	5.96620000
H	-11.94230000	0.29230000	6.48150000
C	-12.97800000	-3.18660000	0.48890000
H	-13.76260000	-2.43850000	0.23610000
H	-13.25570000	-3.68850000	1.44290000
C	-12.90270000	-4.22720000	-0.62490000
H	-12.16780000	-5.01120000	-0.34730000
H	-12.56480000	-3.73890000	-1.56400000
C	-14.25850000	-4.88440000	-0.86350000
H	-14.16750000	-5.64000000	-1.67200000
H	-15.00740000	-4.12380000	-1.17120000
H	-14.60880000	-5.39240000	0.06030000

C	-12.42450000	0.17750000	-0.14820000
H	-12.45230000	-0.68710000	-0.83730000
H	-13.44510000	0.61760000	-0.17850000
C	-11.39030000	1.17840000	-0.61800000
C	-10.07220000	0.77570000	-0.91410000
C	-9.06350000	1.74550000	-1.06630000
C	-9.39990000	3.10720000	-1.05910000
H	-8.59990000	3.82070000	-1.18630000
C	-10.72810000	3.53340000	-0.83980000
C	-11.70890000	2.54450000	-0.61740000
H	-12.72490000	2.83650000	-0.38860000
C	-11.12310000	5.02340000	-0.76490000
C	-11.65710000	5.34040000	0.64950000
H	-11.90680000	6.41940000	0.74400000
H	-10.89150000	5.09020000	1.41600000
H	-12.57820000	4.76480000	0.87880000
C	-12.22190000	5.31980000	-1.80900000
H	-11.86790000	5.05240000	-2.82820000
H	-12.49040000	6.39850000	-1.80400000
H	-13.15030000	4.74830000	-1.60110000
C	-9.94080000	5.98250000	-1.04590000
H	-9.51650000	5.80130000	-2.05720000
H	-9.14100000	5.86230000	-0.28320000
H	-10.27510000	7.04220000	-1.00790000
C	-9.95290000	-1.09530000	-2.24770000
H	-9.36200000	-0.55310000	-3.01900000
H	-11.02530000	-1.05360000	-2.53710000
C	-9.49250000	-2.54750000	-2.20690000
H	-8.38660000	-2.57720000	-2.10960000
H	-9.94280000	-3.03820000	-1.32290000
C	-9.90750000	-3.31550000	-3.45700000
H	-9.53690000	-4.36000000	-3.38830000
H	-9.47730000	-2.84490000	-4.36330000
H	-11.01400000	-3.33680000	-3.54840000
C	-7.61140000	1.33380000	-1.15070000
H	-6.96990000	2.18370000	-1.47050000
H	-7.51110000	0.55330000	-1.92840000
O	-2.57530000	-3.77180000	0.35610000
O	0.78910000	-1.08290000	1.03910000
O	-3.11000000	0.01140000	1.48430000
O	-2.45250000	2.12130000	-3.06650000
O	-2.79890000	-0.53400000	-6.20250000
O	-1.36190000	-3.81730000	-4.10300000
O	3.33710000	-4.48480000	0.19710000
O	5.69230000	-7.20650000	0.94500000
O	6.95350000	-7.22740000	3.91930000

O	5.18720000	-4.44130000	3.55600000
O	1.28800000	4.34440000	0.07380000
O	2.07190000	7.88430000	1.90450000
O	2.53380000	10.35500000	0.12050000
O	2.21560000	7.37930000	-1.62820000
O	-6.31700000	-1.23660000	-0.75050000
O	-8.74240000	-3.41850000	1.38640000
O	-11.70800000	-2.54500000	0.62580000
O	-9.75430000	-0.50890000	-0.95520000
P	1.04820000	-4.04110000	-1.22530000
P	-0.47710000	2.30940000	0.13080000
P	-4.50260000	-1.59890000	-2.76040000
Ir	0.44610000	-0.35850000	-3.09350000
Ir	-0.61470000	-2.32570000	-1.45190000
Ir	-1.21340000	0.27850000	-0.89640000
Ir	-2.23410000	-0.96960000	-3.26780000
C	0.97140000	-1.48480000	-4.53850000
O	1.30030000	-2.15920000	-5.42060000
C	2.05110000	-0.02320000	-2.14710000
O	3.04470000	0.15770000	-1.57370000
C	0.24100000	1.22190000	-5.06370000
H	0.95500000	0.82970000	-5.77940000
H	-0.80180000	1.19170000	-5.34950000
C	0.64990000	1.95420000	-3.98330000
H	-0.07110000	2.53490000	-3.42580000
H	1.70160000	2.15040000	-3.82930000

Π-bound Ethylene at the Basal 1 position on the Tetrairidium-Calixarene complex

0 1

C	-1.95470000	-3.03170000	-0.29340000
C	0.01400000	-0.93480000	0.28270000
C	-2.53210000	0.24140000	0.79290000
C	-2.29130000	1.41570000	-2.22050000
C	-1.36580000	-2.48050000	-3.31500000
C	0.04900000	-5.43650000	-0.74710000
C	0.36550000	-6.11780000	0.44520000
H	1.14940000	-5.76460000	1.09500000
C	-0.32480000	-7.20860000	0.82170000
H	-0.07910000	-7.70510000	1.75090000
C	-1.37380000	-7.70010000	0.03700000
H	-1.92110000	-8.57900000	0.35200000
C	-1.72580000	-7.04320000	-1.14300000
H	-2.54720000	-7.40770000	-1.74600000
C	-1.02240000	-5.90110000	-1.52890000
H	-1.32030000	-5.37560000	-2.42530000
C	1.85360000	-4.16610000	-2.72870000

C	1.63790000	-5.29060000	-3.54470000
H	0.89560000	-6.03090000	-3.29730000
C	2.39330000	-5.47570000	-4.70750000
H	2.21830000	-6.34130000	-5.33330000
C	3.38330000	-4.55410000	-5.05590000
H	3.97370000	-4.70450000	-5.95030000
C	3.61980000	-3.44580000	-4.24090000
H	4.39480000	-2.73680000	-4.50220000
C	2.85450000	-3.24970000	-3.08790000
H	3.05520000	-2.38690000	-2.47130000
C	2.11480000	-3.49310000	0.08980000
H	2.50320000	-2.47780000	-0.13430000
H	1.59200000	-3.45620000	1.06660000
C	4.44780000	-4.03660000	-0.17320000
C	5.14230000	-4.71450000	-1.19430000
C	6.29010000	-4.13750000	-1.75190000
H	6.74630000	-4.61940000	-2.60500000
C	6.86710000	-2.97520000	-1.21950000
C	6.24770000	-2.39050000	-0.09690000
H	6.66480000	-1.50800000	0.36290000
C	5.06340000	-2.91540000	0.45220000
C	8.14690000	-2.40740000	-1.86610000
C	7.80840000	-1.89410000	-3.28100000
H	7.42190000	-2.71170000	-3.92610000
H	8.71170000	-1.47120000	-3.77190000
H	7.03220000	-1.09980000	-3.22900000
C	9.21840000	-3.52010000	-1.96830000
H	8.96930000	-4.25770000	-2.75890000
H	9.29770000	-4.06950000	-1.00780000
H	10.21530000	-3.09980000	-2.22300000
C	8.75700000	-1.23220000	-1.06600000
H	9.69920000	-0.87710000	-1.53690000
H	8.99090000	-1.53980000	-0.02470000
H	8.05850000	-0.37100000	-1.04270000
C	4.68850000	-6.05980000	-1.71960000
H	3.76700000	-6.41650000	-1.21860000
H	4.43350000	-5.94700000	-2.79180000
C	5.80480000	-7.07210000	-1.55350000
C	6.16690000	-7.54870000	-0.27830000
C	7.38850000	-8.22970000	-0.10570000
C	8.17130000	-8.54400000	-1.22730000
H	9.09580000	-9.07520000	-1.05950000
C	7.78330000	-8.15320000	-2.52770000
C	6.59400000	-7.40860000	-2.66360000
H	6.30070000	-7.03710000	-3.63630000
C	8.63600000	-8.45490000	-3.77840000

C	7.78690000	-9.23430000	-4.80700000
H	6.92610000	-8.63400000	-5.16800000
H	7.39470000	-10.17030000	-4.35340000
H	8.39550000	-9.50560000	-5.69690000
C	9.11310000	-7.12680000	-4.40570000
H	8.25980000	-6.50200000	-4.74270000
H	9.75650000	-7.31850000	-5.29170000
H	9.70250000	-6.54200000	-3.66680000
C	9.89170000	-9.30590000	-3.46960000
H	9.60710000	-10.28000000	-3.01590000
H	10.57940000	-8.76610000	-2.78310000
H	10.45970000	-9.52290000	-4.40040000
C	4.35620000	-8.34590000	0.87840000
H	4.82170000	-9.34910000	1.00890000
H	3.71460000	-8.37460000	-0.03030000
C	3.48370000	-8.04140000	2.08820000
H	4.12790000	-7.95240000	2.98380000
H	2.96220000	-7.07610000	1.93050000
C	2.45430000	-9.14140000	2.32500000
H	1.81050000	-8.86680000	3.18700000
H	2.96130000	-10.10270000	2.55320000
H	1.81630000	-9.27380000	1.42580000
C	7.89080000	-8.58530000	1.27680000
H	8.70580000	-9.33950000	1.22060000
H	7.07710000	-9.07230000	1.84930000
C	8.42710000	-7.35550000	1.97740000
C	7.79960000	-6.82810000	3.12410000
C	8.28340000	-5.63330000	3.69580000
C	9.47860000	-5.07610000	3.21800000
H	9.87740000	-4.20810000	3.72310000
C	10.15930000	-5.61660000	2.11150000
C	9.59340000	-6.74680000	1.48210000
H	10.06220000	-7.19540000	0.61930000
C	11.49870000	-4.99040000	1.66470000
C	11.33570000	-3.46630000	1.45170000
H	12.25390000	-3.02590000	1.00630000
H	11.15380000	-2.92970000	2.40580000
H	10.48620000	-3.25800000	0.77410000
C	12.55340000	-5.23320000	2.76370000
H	13.53670000	-4.80790000	2.46680000
H	12.68240000	-6.32270000	2.94260000
H	12.25310000	-4.75810000	3.72190000
C	12.03750000	-5.59380000	0.34460000
H	12.97700000	-5.08780000	0.03290000
H	11.29880000	-5.47080000	-0.47620000
H	12.27460000	-6.67280000	0.46570000

C	7.10240000	-8.32430000	4.80210000
H	7.50010000	-7.69070000	5.62460000
H	7.90440000	-9.03570000	4.49920000
C	5.89800000	-9.10360000	5.33150000
H	6.13030000	-9.48330000	6.35000000
H	5.01940000	-8.42870000	5.41120000
C	5.55580000	-10.29350000	4.43840000
H	4.63520000	-10.78780000	4.81360000
H	6.38540000	-11.03200000	4.44900000
H	5.38260000	-9.96480000	3.39500000
C	7.53470000	-4.90530000	4.78990000
H	6.68250000	-5.49560000	5.18570000
H	8.22020000	-4.74990000	5.65140000
C	7.02620000	-3.58140000	4.25760000
C	5.82840000	-3.51790000	3.51820000
C	5.49450000	-2.30360000	2.84980000
C	6.25720000	-1.15140000	3.10930000
H	5.99980000	-0.23500000	2.59520000
C	7.39080000	-1.17780000	3.94450000
C	7.76910000	-2.41690000	4.49670000
H	8.66110000	-2.50750000	5.09740000
C	8.22350000	0.10730000	4.13980000
C	8.84410000	0.51640000	2.78790000
H	9.45460000	1.43910000	2.89570000
H	8.06210000	0.71490000	2.03000000
H	9.49830000	-0.29490000	2.40060000
C	9.37970000	-0.06260000	5.15530000
H	9.91790000	0.89880000	5.30440000
H	10.12710000	-0.80060000	4.79150000
H	8.99050000	-0.38890000	6.14410000
C	7.31630000	1.24620000	4.65920000
H	7.91070000	2.16640000	4.84720000
H	6.82620000	0.94640000	5.61050000
H	6.52470000	1.51310000	3.92920000
C	3.68220000	-4.51370000	3.68240000
H	3.14890000	-4.80400000	2.75500000
H	3.37220000	-3.49020000	3.99480000
C	3.27900000	-5.45720000	4.81480000
H	3.68500000	-5.07180000	5.77520000
H	3.71180000	-6.46170000	4.64430000
C	1.76170000	-5.58130000	4.92020000
H	1.50200000	-6.25640000	5.76250000
H	1.34390000	-6.00760000	3.98280000
H	1.30510000	-4.58590000	5.10660000
C	4.50620000	-2.23910000	1.69390000
H	4.29060000	-1.18150000	1.42540000

H	3.53310000	-2.63070000	2.00090000
C	-1.84400000	3.60370000	0.98110000
C	-3.12280000	3.42460000	0.58950000
H	-3.40480000	2.59030000	-0.03070000
C	-4.12160000	4.33040000	0.98310000
H	-5.14340000	4.17300000	0.66100000
C	-3.81930000	5.38570000	1.76270000
H	-4.60160000	6.07090000	2.06420000
C	-2.55540000	5.59370000	2.17440000
H	-2.32400000	6.44060000	2.80750000
C	-1.53710000	4.71110000	1.78920000
H	-0.53120000	4.87800000	2.13600000
C	0.41040000	2.02570000	1.97440000
C	-0.22480000	1.99220000	3.22560000
H	-1.27350000	2.24120000	3.31960000
C	0.49000000	1.61700000	4.36780000
H	-0.00290000	1.59840000	5.33120000
C	1.83550000	1.25210000	4.26590000
H	2.38560000	0.95740000	5.15010000
C	2.46790000	1.25900000	3.02070000
H	3.50790000	0.96960000	2.93940000
C	1.75880000	1.64450000	1.87970000
H	2.26040000	1.63420000	0.92320000
C	0.60120000	3.47390000	-0.54790000
H	1.25270000	2.76810000	-1.10010000
H	-0.02700000	4.05340000	-1.25420000
C	2.67570000	4.42240000	0.17650000
C	3.43380000	4.61120000	1.35710000
C	4.81980000	4.37530000	1.33890000
H	5.35390000	4.44960000	2.27290000
C	5.49210000	4.00860000	0.15870000
C	4.74540000	3.94900000	-1.02520000
H	5.24450000	3.73190000	-1.96010000
C	3.37680000	4.24580000	-1.05350000
C	7.00500000	3.72320000	0.10540000
C	7.67340000	4.68780000	-0.90240000
H	7.33650000	5.72940000	-0.71860000
H	7.41240000	4.43280000	-1.95080000
H	8.78130000	4.64850000	-0.82330000
C	7.70350000	3.89940000	1.47570000
H	7.29000000	3.19080000	2.22370000
H	7.58000000	4.93610000	1.85370000
H	8.79350000	3.69740000	1.39410000
C	7.22760000	2.26840000	-0.35630000
H	6.67750000	1.56490000	0.30510000
H	8.30860000	2.01070000	-0.33300000

H	6.86700000	2.10970000	-1.39450000
C	2.78080000	4.90340000	2.69640000
H	1.68820000	4.98480000	2.63550000
H	2.92190000	3.99690000	3.32100000
C	3.42000000	6.10850000	3.38140000
C	3.37000000	7.43910000	2.86100000
C	4.36110000	8.36080000	3.26180000
C	5.27370000	8.02830000	4.27180000
H	6.00390000	8.77240000	4.55190000
C	5.25650000	6.76320000	4.88800000
C	4.31340000	5.82530000	4.43090000
H	4.33310000	4.82340000	4.83790000
C	6.27630000	6.34740000	5.97040000
C	5.52500000	5.90330000	7.24470000
H	4.89600000	5.00780000	7.05940000
H	4.86810000	6.72200000	7.61040000
H	6.24100000	5.64160000	8.05390000
C	7.24100000	7.48990000	6.37080000
H	7.86030000	7.80930000	5.50470000
H	7.93890000	7.15500000	7.16890000
H	6.67740000	8.36360000	6.76380000
C	7.13340000	5.17470000	5.44320000
H	7.64530000	5.46340000	4.49970000
H	6.51640000	4.27490000	5.24100000
H	7.90750000	4.88560000	6.18680000
C	1.11820000	7.40980000	2.06380000
H	0.87440000	6.97140000	3.05790000
H	0.95970000	6.66510000	1.26460000
C	0.15180000	8.56810000	1.81640000
H	0.44850000	9.11290000	0.89780000
H	-0.87040000	8.16310000	1.65750000
C	0.11940000	9.54290000	2.99040000
H	-0.59010000	10.36730000	2.76770000
H	1.12470000	9.97940000	3.16230000
H	-0.21760000	9.02470000	3.91330000
C	4.45610000	9.72120000	2.60380000
H	3.44220000	10.16150000	2.52610000
H	5.04250000	10.43110000	3.22740000
C	5.12760000	9.58360000	1.25830000
C	4.41040000	9.71290000	0.05200000
C	5.03130000	9.37170000	-1.16530000
C	6.40080000	9.05130000	-1.17820000
H	6.85610000	8.84640000	-2.13500000
C	7.16980000	9.04890000	0.00690000
C	6.49840000	9.29160000	1.22020000
H	7.04340000	9.27810000	2.15380000

C	8.70470000	8.86970000	0.00770000
C	9.35820000	10.21040000	0.40050000
H	9.06480000	11.00880000	-0.31520000
H	10.46660000	10.12550000	0.39520000
H	9.04570000	10.52630000	1.41880000
C	9.26520000	8.45200000	-1.37390000
H	9.09400000	9.24620000	-2.13220000
H	8.79580000	7.50680000	-1.72110000
H	10.36310000	8.28560000	-1.32160000
C	9.12810000	7.78890000	1.03040000
H	8.58300000	6.84520000	0.84660000
H	8.93300000	8.10400000	2.07590000
H	10.21730000	7.57930000	0.95800000
C	3.06420000	11.64190000	0.09290000
H	3.60700000	12.06850000	-0.78100000
H	3.56220000	12.01070000	1.01660000
C	1.61790000	12.14020000	0.10100000
H	1.60040000	13.19130000	0.46220000
H	1.01340000	11.52980000	0.80470000
C	0.98950000	12.10080000	-1.28970000
H	-0.06700000	12.43650000	-1.22880000
H	1.00980000	11.07480000	-1.70400000
H	1.53740000	12.77880000	-1.97810000
C	4.27090000	9.39790000	-2.47350000
H	4.78040000	10.11830000	-3.14980000
H	3.24520000	9.79510000	-2.35720000
C	4.22640000	8.01770000	-3.09860000
C	3.39550000	6.99470000	-2.58610000
C	3.52320000	5.68230000	-3.07590000
C	4.40240000	5.41600000	-4.13370000
H	4.48350000	4.39910000	-4.49330000
C	5.20710000	6.42620000	-4.69600000
C	5.10080000	7.72800000	-4.15980000
H	5.72160000	8.52970000	-4.52970000
C	6.19930000	6.06550000	-5.82200000
C	7.00080000	7.28330000	-6.34270000
H	7.68670000	6.98190000	-7.16420000
H	7.62640000	7.72210000	-5.53530000
H	6.31860000	8.06270000	-6.74590000
C	5.42750000	5.46890000	-7.01960000
H	6.11760000	5.24490000	-7.86180000
H	4.65870000	6.18660000	-7.37920000
H	4.91950000	4.52000000	-6.74890000
C	7.21520000	5.02780000	-5.29550000
H	7.96680000	4.78060000	-6.07640000
H	6.71830000	4.08000000	-5.00080000

H	7.75200000	5.42940000	-4.40860000
C	1.31850000	7.98990000	-1.95160000
H	1.38540000	8.37020000	-2.99770000
H	1.23700000	8.86080000	-1.27670000
C	0.05760000	7.13360000	-1.82080000
H	0.05380000	6.60730000	-0.84560000
H	0.04090000	6.37510000	-2.63090000
C	-1.20510000	7.98330000	-1.92540000
H	-2.09930000	7.33030000	-1.84120000
H	-1.23640000	8.50810000	-2.90390000
H	-1.23640000	8.73280000	-1.10610000
C	2.77900000	4.54100000	-2.41640000
H	2.83780000	3.61820000	-3.03270000
H	1.72080000	4.83310000	-2.36960000
C	-5.66120000	-0.32950000	-3.87840000
C	-5.70510000	1.07250000	-3.84760000
H	-5.02910000	1.62610000	-3.21300000
C	-6.63640000	1.77270000	-4.61890000
H	-6.66370000	2.85400000	-4.58390000
C	-7.53530000	1.07750000	-5.42870000
H	-8.25640000	1.61910000	-6.02690000
C	-7.50960000	-0.31810000	-5.45850000
H	-8.21210000	-0.85460000	-6.08240000
C	-6.58810000	-1.02220000	-4.67610000
H	-6.62040000	-2.09990000	-4.69280000
C	-4.63690000	-3.00410000	-3.07200000
C	-4.47870000	-3.59240000	-4.33690000
H	-4.31580000	-2.98750000	-5.21430000
C	-4.53870000	-4.98570000	-4.47390000
H	-4.42140000	-5.43220000	-5.45320000
C	-4.72650000	-5.77240000	-3.39890000
H	-4.75660000	-6.84760000	-3.52350000
C	-4.86980000	-5.24500000	-2.17000000
H	-5.00080000	-5.89730000	-1.31660000
C	-4.83920000	-3.85810000	-1.97960000
H	-4.93560000	-3.47450000	-0.98400000
C	-4.90110000	-0.76540000	-1.13490000
H	-4.28210000	-1.35170000	-0.43020000
H	-4.65150000	0.31190000	-1.01330000
C	-6.68210000	-0.30080000	0.29970000
C	-6.36020000	-0.81050000	1.57720000
C	-6.37580000	0.05080000	2.68450000
H	-6.03600000	-0.32830000	3.63740000
C	-6.79630000	1.38760000	2.58020000
C	-7.25250000	1.83440000	1.32340000
H	-7.61740000	2.84170000	1.19050000

C	-7.20920000	1.00330000	0.19150000
C	-6.72950000	2.29890000	3.82320000
C	-5.25410000	2.47050000	4.24520000
H	-4.65970000	2.90320000	3.41330000
H	-4.79540000	1.49840000	4.52410000
H	-5.17170000	3.14700000	5.12340000
C	-7.51750000	1.65320000	4.98610000
H	-8.52750000	1.34880000	4.64630000
H	-7.62650000	2.35880000	5.83790000
H	-7.00340000	0.75090000	5.37630000
C	-7.31890000	3.70820000	3.57400000
H	-8.38380000	3.64260000	3.26420000
H	-6.74260000	4.24800000	2.79220000
H	-7.27410000	4.32420000	4.49820000
C	-5.98310000	-2.25800000	1.79800000
H	-5.91720000	-2.80080000	0.85040000
H	-4.95480000	-2.28960000	2.21970000
C	-6.97610000	-2.91350000	2.74730000
C	-8.31620000	-3.19440000	2.35960000
C	-9.31200000	-3.26780000	3.35220000
C	-8.94970000	-3.28230000	4.70530000
H	-9.73000000	-3.38770000	5.44690000
C	-7.60820000	-3.15940000	5.11200000
C	-6.63400000	-2.96320000	4.11050000
H	-5.60640000	-2.76580000	4.37570000
C	-7.26790000	-3.18110000	6.61780000
C	-8.01270000	-2.03270000	7.33500000
H	-9.11400000	-2.15680000	7.27780000
H	-7.74930000	-1.05590000	6.87700000
H	-7.73960000	-1.99780000	8.41200000
C	-7.70730000	-4.53260000	7.22170000
H	-8.80520000	-4.67690000	7.14510000
H	-7.43930000	-4.58940000	8.29910000
H	-7.20750000	-5.37260000	6.69250000
C	-5.75630000	-3.00930000	6.90390000
H	-5.16730000	-3.81910000	6.42120000
H	-5.55400000	-3.05500000	7.99620000
H	-5.39370000	-2.02270000	6.54180000
C	-7.90940000	-4.27440000	0.29230000
H	-7.06590000	-4.74250000	0.85040000
H	-7.50540000	-3.71610000	-0.57640000
C	-8.80980000	-5.40640000	-0.20320000
H	-9.16610000	-5.99900000	0.66710000
H	-9.69540000	-4.98420000	-0.71540000
C	-8.07870000	-6.32760000	-1.17290000
H	-8.76660000	-7.13070000	-1.51110000

H	-7.20570000	-6.79750000	-0.67310000
H	-7.73890000	-5.75660000	-2.06290000
C	-10.77450000	-3.37190000	2.97700000
H	-10.89190000	-4.08330000	2.13290000
H	-11.36550000	-3.80780000	3.81210000
C	-11.33320000	-2.00230000	2.65760000
C	-11.74010000	-1.65570000	1.35330000
C	-12.19310000	-0.34740000	1.08750000
C	-12.34950000	0.55770000	2.14670000
H	-12.75300000	1.53710000	1.92930000
C	-11.98260000	0.22730000	3.46410000
C	-11.45850000	-1.06290000	3.69570000
H	-11.15680000	-1.36950000	4.68560000
C	-12.18080000	1.26670000	4.58800000
C	-11.48490000	2.59530000	4.20740000
H	-11.99630000	3.10210000	3.36290000
H	-10.43410000	2.41100000	3.90850000
H	-11.48890000	3.30730000	5.06080000
C	-13.69040000	1.52300000	4.77570000
H	-14.14970000	1.92960000	3.84970000
H	-13.86650000	2.25730000	5.59170000
H	-14.21400000	0.57760000	5.03590000
C	-11.60400000	0.80500000	5.94880000
H	-11.73050000	1.59520000	6.72040000 0 1
C	-1.95470000	-3.03170000	-0.29340000
C	0.01400000	-0.93480000	0.28270000
C	-2.53210000	0.24140000	0.79290000
C	-2.29130000	1.41570000	-2.22050000
C	-1.36580000	-2.48050000	-3.31500000
C	0.04900000	-5.43650000	-0.74710000
C	0.36550000	-6.11780000	0.44520000
H	1.14940000	-5.76460000	1.09500000
C	-0.32480000	-7.20860000	0.82170000
H	-0.07910000	-7.70510000	1.75090000
C	-1.37380000	-7.70010000	0.03700000
H	-1.92110000	-8.57900000	0.35200000
C	-1.72580000	-7.04320000	-1.14300000
H	-2.54720000	-7.40770000	-1.74600000
C	-1.02240000	-5.90110000	-1.52890000
H	-1.32030000	-5.37560000	-2.42530000
C	1.85360000	-4.16610000	-2.72870000
C	1.63790000	-5.29060000	-3.54470000
H	0.89560000	-6.03090000	-3.29730000
C	2.39330000	-5.47570000	-4.70750000
H	2.21830000	-6.34130000	-5.33330000
C	3.38330000	-4.55410000	-5.05590000

H	3.97370000	-4.70450000	-5.95030000
C	3.61980000	-3.44580000	-4.24090000
H	4.39480000	-2.73680000	-4.50220000
C	2.85450000	-3.24970000	-3.08790000
H	3.05520000	-2.38690000	-2.47130000
C	2.11480000	-3.49310000	0.08980000
H	2.50320000	-2.47780000	-0.13430000
H	1.59200000	-3.45620000	1.06660000
C	4.44780000	-4.03660000	-0.17320000
C	5.14230000	-4.71450000	-1.19430000
C	6.29010000	-4.13750000	-1.75190000
H	6.74630000	-4.61940000	-2.60500000
C	6.86710000	-2.97520000	-1.21950000
C	6.24770000	-2.39050000	-0.09690000
H	6.66480000	-1.50800000	0.36290000
C	5.06340000	-2.91540000	0.45220000
C	8.14690000	-2.40740000	-1.86610000
C	7.80840000	-1.89410000	-3.28100000
H	7.42190000	-2.71170000	-3.92610000
H	8.71170000	-1.47120000	-3.77190000
H	7.03220000	-1.09980000	-3.22900000
C	9.21840000	-3.52010000	-1.96830000
H	8.96930000	-4.25770000	-2.75890000
H	9.29770000	-4.06950000	-1.00780000
H	10.21530000	-3.09980000	-2.22300000
C	8.75700000	-1.23220000	-1.06600000
H	9.69920000	-0.87710000	-1.53690000
H	8.99090000	-1.53980000	-0.02470000
H	8.05850000	-0.37100000	-1.04270000
C	4.68850000	-6.05980000	-1.71960000
H	3.76700000	-6.41650000	-1.21860000
H	4.43350000	-5.94700000	-2.79180000
C	5.80480000	-7.07210000	-1.55350000
C	6.16690000	-7.54870000	-0.27830000
C	7.38850000	-8.22970000	-0.10570000
C	8.17130000	-8.54400000	-1.22730000
H	9.09580000	-9.07520000	-1.05950000
C	7.78330000	-8.15320000	-2.52770000
C	6.59400000	-7.40860000	-2.66360000
H	6.30070000	-7.03710000	-3.63630000
C	8.63600000	-8.45490000	-3.77840000
C	7.78690000	-9.23430000	-4.80700000
H	6.92610000	-8.63400000	-5.16800000
H	7.39470000	-10.17030000	-4.35340000
H	8.39550000	-9.50560000	-5.69690000
C	9.11310000	-7.12680000	-4.40570000

H	8.25980000	-6.50200000	-4.74270000
H	9.75650000	-7.31850000	-5.29170000
H	9.70250000	-6.54200000	-3.66680000
C	9.89170000	-9.30590000	-3.46960000
H	9.60710000	-10.28000000	-3.01590000
H	10.57940000	-8.76610000	-2.78310000
H	10.45970000	-9.52290000	-4.40040000
C	4.35620000	-8.34590000	0.87840000
H	4.82170000	-9.34910000	1.00890000
H	3.71460000	-8.37460000	-0.03030000
C	3.48370000	-8.04140000	2.08820000
H	4.12790000	-7.95240000	2.98380000
H	2.96220000	-7.07610000	1.93050000
C	2.45430000	-9.14140000	2.32500000
H	1.81050000	-8.86680000	3.18700000
H	2.96130000	-10.10270000	2.55320000
H	1.81630000	-9.27380000	1.42580000
C	7.89080000	-8.58530000	1.27680000
H	8.70580000	-9.33950000	1.22060000
H	7.07710000	-9.07230000	1.84930000
C	8.42710000	-7.35550000	1.97740000
C	7.79960000	-6.82810000	3.12410000
C	8.28340000	-5.63330000	3.69580000
C	9.47860000	-5.07610000	3.21800000
H	9.87740000	-4.20810000	3.72310000
C	10.15930000	-5.61660000	2.11150000
C	9.59340000	-6.74680000	1.48210000
H	10.06220000	-7.19540000	0.61930000
C	11.49870000	-4.99040000	1.66470000
C	11.33570000	-3.46630000	1.45170000
H	12.25390000	-3.02590000	1.00630000
H	11.15380000	-2.92970000	2.40580000
H	10.48620000	-3.25800000	0.77410000
C	12.55340000	-5.23320000	2.76370000
H	13.53670000	-4.80790000	2.46680000
H	12.68240000	-6.32270000	2.94260000
H	12.25310000	-4.75810000	3.72190000
C	12.03750000	-5.59380000	0.34460000
H	12.97700000	-5.08780000	0.03290000
H	11.29880000	-5.47080000	-0.47620000
H	12.27460000	-6.67280000	0.46570000
C	7.10240000	-8.32430000	4.80210000
H	7.50010000	-7.69070000	5.62460000
H	7.90440000	-9.03570000	4.49920000
C	5.89800000	-9.10360000	5.33150000
H	6.13030000	-9.48330000	6.35000000

H	5.01940000	-8.42870000	5.41120000
C	5.55580000	-10.29350000	4.43840000
H	4.63520000	-10.78780000	4.81360000
H	6.38540000	-11.03200000	4.44900000
H	5.38260000	-9.96480000	3.39500000
C	7.53470000	-4.90530000	4.78990000
H	6.68250000	-5.49560000	5.18570000
H	8.22020000	-4.74990000	5.65140000
C	7.02620000	-3.58140000	4.25760000
C	5.82840000	-3.51790000	3.51820000
C	5.49450000	-2.30360000	2.84980000
C	6.25720000	-1.15140000	3.10930000
H	5.99980000	-0.23500000	2.59520000
C	7.39080000	-1.17780000	3.94450000
C	7.76910000	-2.41690000	4.49670000
H	8.66110000	-2.50750000	5.09740000
C	8.22350000	0.10730000	4.13980000
C	8.84410000	0.51640000	2.78790000
H	9.45460000	1.43910000	2.89570000
H	8.06210000	0.71490000	2.03000000
H	9.49830000	-0.29490000	2.40060000
C	9.37970000	-0.06260000	5.15530000
H	9.91790000	0.89880000	5.30440000
H	10.12710000	-0.80060000	4.79150000
H	8.99050000	-0.38890000	6.14410000
C	7.31630000	1.24620000	4.65920000
H	7.91070000	2.16640000	4.84720000
H	6.82620000	0.94640000	5.61050000
H	6.52470000	1.51310000	3.92920000
C	3.68220000	-4.51370000	3.68240000
H	3.14890000	-4.80400000	2.75500000
H	3.37220000	-3.49020000	3.99480000
C	3.27900000	-5.45720000	4.81480000
H	3.68500000	-5.07180000	5.77520000
H	3.71180000	-6.46170000	4.64430000
C	1.76170000	-5.58130000	4.92020000
H	1.50200000	-6.25640000	5.76250000
H	1.34390000	-6.00760000	3.98280000
H	1.30510000	-4.58590000	5.10660000
C	4.50620000	-2.23910000	1.69390000
H	4.29060000	-1.18150000	1.42540000
H	3.53310000	-2.63070000	2.00090000
C	-1.84400000	3.60370000	0.98110000
C	-3.12280000	3.42460000	0.58950000
H	-3.40480000	2.59030000	-0.03070000
C	-4.12160000	4.33040000	0.98310000

H	-5.14340000	4.17300000	0.66100000
C	-3.81930000	5.38570000	1.76270000
H	-4.60160000	6.07090000	2.06420000
C	-2.55540000	5.59370000	2.17440000
H	-2.32400000	6.44060000	2.80750000
C	-1.53710000	4.71110000	1.78920000
H	-0.53120000	4.87800000	2.13600000
C	0.41040000	2.02570000	1.97440000
C	-0.22480000	1.99220000	3.22560000
H	-1.27350000	2.24120000	3.31960000
C	0.49000000	1.61700000	4.36780000
H	-0.00290000	1.59840000	5.33120000
C	1.83550000	1.25210000	4.26590000
H	2.38560000	0.95740000	5.15010000
C	2.46790000	1.25900000	3.02070000
H	3.50790000	0.96960000	2.93940000
C	1.75880000	1.64450000	1.87970000
H	2.26040000	1.63420000	0.92320000
C	0.60120000	3.47390000	-0.54790000
H	1.25270000	2.76810000	-1.10010000
H	-0.02700000	4.05340000	-1.25420000
C	2.67570000	4.42240000	0.17650000
C	3.43380000	4.61120000	1.35710000
C	4.81980000	4.37530000	1.33890000
H	5.35390000	4.44960000	2.27290000
C	5.49210000	4.00860000	0.15870000
C	4.74540000	3.94900000	-1.02520000
H	5.24450000	3.73190000	-1.96010000
C	3.37680000	4.24580000	-1.05350000
C	7.00500000	3.72320000	0.10540000
C	7.67340000	4.68780000	-0.90240000
H	7.33650000	5.72940000	-0.71860000
H	7.41240000	4.43280000	-1.95080000
H	8.78130000	4.64850000	-0.82330000
C	7.70350000	3.89940000	1.47570000
H	7.29000000	3.19080000	2.22370000
H	7.58000000	4.93610000	1.85370000
H	8.79350000	3.69740000	1.39410000
C	7.22760000	2.26840000	-0.35630000
H	6.67750000	1.56490000	0.30510000
H	8.30860000	2.01070000	-0.33300000
H	6.86700000	2.10970000	-1.39450000
C	2.78080000	4.90340000	2.69640000
H	1.68820000	4.98480000	2.63550000
H	2.92190000	3.99690000	3.32100000
C	3.42000000	6.10850000	3.38140000

C	3.37000000	7.43910000	2.86100000
C	4.36110000	8.36080000	3.26180000
C	5.27370000	8.02830000	4.27180000
H	6.00390000	8.77240000	4.55190000
C	5.25650000	6.76320000	4.88800000
C	4.31340000	5.82530000	4.43090000
H	4.33310000	4.82340000	4.83790000
C	6.27630000	6.34740000	5.97040000
C	5.52500000	5.90330000	7.24470000
H	4.89600000	5.00780000	7.05940000
H	4.86810000	6.72200000	7.61040000
H	6.24100000	5.64160000	8.05390000
C	7.24100000	7.48990000	6.37080000
H	7.86030000	7.80930000	5.50470000
H	7.93890000	7.15500000	7.16890000
H	6.67740000	8.36360000	6.76380000
C	7.13340000	5.17470000	5.44320000
H	7.64530000	5.46340000	4.49970000
H	6.51640000	4.27490000	5.24100000
H	7.90750000	4.88560000	6.18680000
C	1.11820000	7.40980000	2.06380000
H	0.87440000	6.97140000	3.05790000
H	0.95970000	6.66510000	1.26460000
C	0.15180000	8.56810000	1.81640000
H	0.44850000	9.11290000	0.89780000
H	-0.87040000	8.16310000	1.65750000
C	0.11940000	9.54290000	2.99040000
H	-0.59010000	10.36730000	2.76770000
H	1.12470000	9.97940000	3.16230000
H	-0.21760000	9.02470000	3.91330000
C	4.45610000	9.72120000	2.60380000
H	3.44220000	10.16150000	2.52610000
H	5.04250000	10.43110000	3.22740000
C	5.12760000	9.58360000	1.25830000
C	4.41040000	9.71290000	0.05200000
C	5.03130000	9.37170000	-1.16530000
C	6.40080000	9.05130000	-1.17820000
H	6.85610000	8.84640000	-2.13500000
C	7.16980000	9.04890000	0.00690000
C	6.49840000	9.29160000	1.22020000
H	7.04340000	9.27810000	2.15380000
C	8.70470000	8.86970000	0.00770000
C	9.35820000	10.21040000	0.40050000
H	9.06480000	11.00880000	-0.31520000
H	10.46660000	10.12550000	0.39520000
H	9.04570000	10.52630000	1.41880000

C	9.26520000	8.45200000	-1.37390000
H	9.09400000	9.24620000	-2.13220000
H	8.79580000	7.50680000	-1.72110000
H	10.36310000	8.28560000	-1.32160000
C	9.12810000	7.78890000	1.03040000
H	8.58300000	6.84520000	0.84660000
H	8.93300000	8.10400000	2.07590000
H	10.21730000	7.57930000	0.95800000
C	3.06420000	11.64190000	0.09290000
H	3.60700000	12.06850000	-0.78100000
H	3.56220000	12.01070000	1.01660000
C	1.61790000	12.14020000	0.10100000
H	1.60040000	13.19130000	0.46220000
H	1.01340000	11.52980000	0.80470000
C	0.98950000	12.10080000	-1.28970000
H	-0.06700000	12.43650000	-1.22880000
H	1.00980000	11.07480000	-1.70400000
H	1.53740000	12.77880000	-1.97810000
C	4.27090000	9.39790000	-2.47350000
H	4.78040000	10.11830000	-3.14980000
H	3.24520000	9.79510000	-2.35720000
C	4.22640000	8.01770000	-3.09860000
C	3.39550000	6.99470000	-2.58610000
C	3.52320000	5.68230000	-3.07590000
C	4.40240000	5.41600000	-4.13370000
H	4.48350000	4.39910000	-4.49330000
C	5.20710000	6.42620000	-4.69600000
C	5.10080000	7.72800000	-4.15980000
H	5.72160000	8.52970000	-4.52970000
C	6.19930000	6.06550000	-5.82200000
C	7.00080000	7.28330000	-6.34270000
H	7.68670000	6.98190000	-7.16420000
H	7.62640000	7.72210000	-5.53530000
H	6.31860000	8.06270000	-6.74590000
C	5.42750000	5.46890000	-7.01960000
H	6.11760000	5.24490000	-7.86180000
H	4.65870000	6.18660000	-7.37920000
H	4.91950000	4.52000000	-6.74890000
C	7.21520000	5.02780000	-5.29550000
H	7.96680000	4.78060000	-6.07640000
H	6.71830000	4.08000000	-5.00080000
H	7.75200000	5.42940000	-4.40860000
C	1.31850000	7.98990000	-1.95160000
H	1.38540000	8.37020000	-2.99770000
H	1.23700000	8.86080000	-1.27670000
C	0.05760000	7.13360000	-1.82080000

H	0.05380000	6.60730000	-0.84560000
H	0.04090000	6.37510000	-2.63090000
C	-1.20510000	7.98330000	-1.92540000
H	-2.09930000	7.33030000	-1.84120000
H	-1.23640000	8.50810000	-2.90390000
H	-1.23640000	8.73280000	-1.10610000
C	2.77900000	4.54100000	-2.41640000
H	2.83780000	3.61820000	-3.03270000
H	1.72080000	4.83310000	-2.36960000
C	-5.66120000	-0.32950000	-3.87840000
C	-5.70510000	1.07250000	-3.84760000
H	-5.02910000	1.62610000	-3.21300000
C	-6.63640000	1.77270000	-4.61890000
H	-6.66370000	2.85400000	-4.58390000
C	-7.53530000	1.07750000	-5.42870000
H	-8.25640000	1.61910000	-6.02690000
C	-7.50960000	-0.31810000	-5.45850000
H	-8.21210000	-0.85460000	-6.08240000
C	-6.58810000	-1.02220000	-4.67610000
H	-6.62040000	-2.09990000	-4.69280000
C	-4.63690000	-3.00410000	-3.07200000
C	-4.47870000	-3.59240000	-4.33690000
H	-4.31580000	-2.98750000	-5.21430000
C	-4.53870000	-4.98570000	-4.47390000
H	-4.42140000	-5.43220000	-5.45320000
C	-4.72650000	-5.77240000	-3.39890000
H	-4.75660000	-6.84760000	-3.52350000
C	-4.86980000	-5.24500000	-2.17000000
H	-5.00080000	-5.89730000	-1.31660000
C	-4.83920000	-3.85810000	-1.97960000
H	-4.93560000	-3.47450000	-0.98400000
C	-4.90110000	-0.76540000	-1.13490000
H	-4.28210000	-1.35170000	-0.43020000
H	-4.65150000	0.31190000	-1.01330000
C	-6.68210000	-0.30080000	0.29970000
C	-6.36020000	-0.81050000	1.57720000
C	-6.37580000	0.05080000	2.68450000
H	-6.03600000	-0.32830000	3.63740000
C	-6.79630000	1.38760000	2.58020000
C	-7.25250000	1.83440000	1.32340000
H	-7.61740000	2.84170000	1.19050000
C	-7.20920000	1.00330000	0.19150000
C	-6.72950000	2.29890000	3.82320000
C	-5.25410000	2.47050000	4.24520000
H	-4.65970000	2.90320000	3.41330000
H	-4.79540000	1.49840000	4.52410000

H	-5.17170000	3.14700000	5.12340000
C	-7.51750000	1.65320000	4.98610000
H	-8.52750000	1.34880000	4.64630000
H	-7.62650000	2.35880000	5.83790000
H	-7.00340000	0.75090000	5.37630000
C	-7.31890000	3.70820000	3.57400000
H	-8.38380000	3.64260000	3.26420000
H	-6.74260000	4.24800000	2.79220000
H	-7.27410000	4.32420000	4.49820000
C	-5.98310000	-2.25800000	1.79800000
H	-5.91720000	-2.80080000	0.85040000
H	-4.95480000	-2.28960000	2.21970000
C	-6.97610000	-2.91350000	2.74730000
C	-8.31620000	-3.19440000	2.35960000
C	-9.31200000	-3.26780000	3.35220000
C	-8.94970000	-3.28230000	4.70530000
H	-9.73000000	-3.38770000	5.44690000
C	-7.60820000	-3.15940000	5.11200000
C	-6.63400000	-2.96320000	4.11050000
H	-5.60640000	-2.76580000	4.37570000
C	-7.26790000	-3.18110000	6.61780000
C	-8.01270000	-2.03270000	7.33500000
H	-9.11400000	-2.15680000	7.27780000
H	-7.74930000	-1.05590000	6.87700000
H	-7.73960000	-1.99780000	8.41200000
C	-7.70730000	-4.53260000	7.22170000
H	-8.80520000	-4.67690000	7.14510000
H	-7.43930000	-4.58940000	8.29910000
H	-7.20750000	-5.37260000	6.69250000
C	-5.75630000	-3.00930000	6.90390000
H	-5.16730000	-3.81910000	6.42120000
H	-5.55400000	-3.05500000	7.99620000
H	-5.39370000	-2.02270000	6.54180000
C	-7.90940000	-4.27440000	0.29230000
H	-7.06590000	-4.74250000	0.85040000
H	-7.50540000	-3.71610000	-0.57640000
C	-8.80980000	-5.40640000	-0.20320000
H	-9.16610000	-5.99900000	0.66710000
H	-9.69540000	-4.98420000	-0.71540000
C	-8.07870000	-6.32760000	-1.17290000
H	-8.76660000	-7.13070000	-1.51110000
H	-7.20570000	-6.79750000	-0.67310000
H	-7.73890000	-5.75660000	-2.06290000
C	-10.77450000	-3.37190000	2.97700000
H	-10.89190000	-4.08330000	2.13290000
H	-11.36550000	-3.80780000	3.81210000

C	-11.33320000	-2.00230000	2.65760000
C	-11.74010000	-1.65570000	1.35330000
C	-12.19310000	-0.34740000	1.08750000
C	-12.34950000	0.55770000	2.14670000
H	-12.75300000	1.53710000	1.92930000
C	-11.98260000	0.22730000	3.46410000
C	-11.45850000	-1.06290000	3.69570000
H	-11.15680000	-1.36950000	4.68560000
C	-12.18080000	1.26670000	4.58800000
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H	-11.99630000	3.10210000	3.36290000
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H	-11.48890000	3.30730000	5.06080000
C	-13.69040000	1.52300000	4.77570000
H	-14.14970000	1.92960000	3.84970000
H	-13.86650000	2.25730000	5.59170000
H	-14.21400000	0.57760000	5.03590000
C	-11.60400000	0.80500000	5.94880000
H	-11.73050000	1.59520000	6.72040000
H	-10.51820000	0.58600000	5.86490000
H	-12.13190000	-0.10010000	6.31910000
C	-12.91540000	-3.27550000	0.11430000
H	-13.71840000	-2.54070000	-0.11890000
H	-13.20100000	-3.83880000	1.03100000
C	-12.77530000	-4.24960000	-1.05230000
H	-12.03110000	-5.03060000	-0.79240000
H	-12.41780000	-3.70150000	-1.95050000
C	-14.10480000	-4.92440000	-1.37510000
H	-13.96640000	-5.63190000	-2.21950000
H	-14.86170000	-4.16590000	-1.66810000
H	-14.47400000	-5.49060000	-0.49350000
C	-12.47800000	0.13180000	-0.31860000
H	-12.44940000	-0.69180000	-1.05600000
H	-13.51600000	0.52900000	-0.35250000
C	-11.47720000	1.20140000	-0.70090000
C	-10.13530000	0.87330000	-0.98180000
C	-9.16660000	1.89230000	-1.04820000
C	-9.56260000	3.23570000	-0.97000000
H	-8.79200000	3.98890000	-1.03420000
C	-10.91390000	3.59130000	-0.76550000
C	-11.85550000	2.55020000	-0.62970000
H	-12.88920000	2.78470000	-0.41430000
C	-11.37700000	5.05610000	-0.61910000
C	-11.96400000	5.26820000	0.79390000
H	-12.26480000	6.32830000	0.94080000
H	-11.20960000	5.00830000	1.56810000

H	-12.86420000	4.64110000	0.96260000
C	-12.45850000	5.36420000	-1.67790000
H	-12.06460000	5.17100000	-2.69920000
H	-12.77490000	6.42840000	-1.62080000
H	-13.36590000	4.74250000	-1.53060000
C	-10.23150000	6.07980000	-0.80990000
H	-9.77200000	5.97570000	-1.81670000
H	-9.44840000	5.95000000	-0.03170000
H	-10.61370000	7.12010000	-0.72220000
C	-9.90420000	-0.90450000	-2.42450000
H	-9.32190000	-0.28990000	-3.14680000
H	-10.97070000	-0.89220000	-2.73720000
C	-9.37870000	-2.33450000	-2.46190000
H	-8.27510000	-2.32130000	-2.33800000
H	-9.82710000	-2.89930000	-1.62220000
C	-9.72900000	-3.03910000	-3.76780000
H	-9.30880000	-4.06700000	-3.75660000
H	-9.30340000	-2.49080000	-4.63170000
H	-10.83100000	-3.10730000	-3.88670000
C	-7.69690000	1.54810000	-1.13090000
H	-7.08840000	2.44110000	-1.39260000
H	-7.55640000	0.81650000	-1.94760000
O	-2.69390000	-3.57490000	0.41650000
O	0.68250000	-1.04810000	1.24720000
O	-3.20200000	0.08570000	1.72660000
O	-2.66220000	2.49490000	-2.51490000
O	-1.30300000	-3.34490000	-4.11540000
O	3.15230000	-4.48250000	0.15430000
O	5.37320000	-7.34240000	0.76070000
O	6.71280000	-7.50320000	3.69570000
O	5.09410000	-4.62850000	3.45790000
O	1.34460000	4.36620000	0.29850000
O	2.46510000	7.88530000	1.98700000
O	3.09970000	10.21070000	0.05510000
O	2.47590000	7.24340000	-1.55490000
O	-6.29140000	-0.98430000	-0.86700000
O	-8.69530000	-3.38040000	1.09630000
O	-11.67230000	-2.60110000	0.32260000
O	-9.76070000	-0.39170000	-1.09370000
P	0.87270000	-3.86930000	-1.21420000
P	-0.52820000	2.43980000	0.46420000
P	-4.41450000	-1.19600000	-2.85610000
Ir	0.54840000	0.03730000	-2.71260000
Ir	-0.71240000	-2.08630000	-1.34520000
Ir	-1.28790000	0.46800000	-0.61300000
Ir	-2.14980000	-0.51120000	-3.17070000

C	1.02340000	-0.94290000	-4.29150000
O	1.29670000	-1.46370000	-5.28770000
C	2.16050000	0.09380000	-1.66380000
O	3.17200000	0.14670000	-1.10290000
C	0.43110000	1.79420000	-3.47300000
O	0.38100000	2.83030000	-3.98530000
C	-2.31200000	-0.63440000	-5.37220000
H	-1.38930000	-1.04370000	-5.76880000
H	-3.20560000	-1.13520000	-5.72590000
C	-2.39310000	0.71890000	-4.98800000
H	-3.33580000	1.25090000	-5.02540000
H	-1.52750000	1.36220000	-5.08380000
H	-10.51820000	0.58600000	5.86490000
H	-12.13190000	-0.10010000	6.31910000
C	-12.91540000	-3.27550000	0.11430000
H	-13.71840000	-2.54070000	-0.11890000
H	-13.20100000	-3.83880000	1.03100000
C	-12.77530000	-4.24960000	-1.05230000
H	-12.03110000	-5.03060000	-0.79240000
H	-12.41780000	-3.70150000	-1.95050000
C	-14.10480000	-4.92440000	-1.37510000
H	-13.96640000	-5.63190000	-2.21950000
H	-14.86170000	-4.16590000	-1.66810000
H	-14.47400000	-5.49060000	-0.49350000
C	-12.47800000	0.13180000	-0.31860000
H	-12.44940000	-0.69180000	-1.05600000
H	-13.51600000	0.52900000	-0.35250000
C	-11.47720000	1.20140000	-0.70090000
C	-10.13530000	0.87330000	-0.98180000
C	-9.16660000	1.89230000	-1.04820000
C	-9.56260000	3.23570000	-0.97000000
H	-8.79200000	3.98890000	-1.03420000
C	-10.91390000	3.59130000	-0.76550000
C	-11.85550000	2.55020000	-0.62970000
H	-12.88920000	2.78470000	-0.41430000
C	-11.37700000	5.05610000	-0.61910000
C	-11.96400000	5.26820000	0.79390000
H	-12.26480000	6.32830000	0.94080000
H	-11.20960000	5.00830000	1.56810000
H	-12.86420000	4.64110000	0.96260000
C	-12.45850000	5.36420000	-1.67790000
H	-12.06460000	5.17100000	-2.69920000
H	-12.77490000	6.42840000	-1.62080000
H	-13.36590000	4.74250000	-1.53060000
C	-10.23150000	6.07980000	-0.80990000
H	-9.77200000	5.97570000	-1.81670000

H	-9.44840000	5.95000000	-0.03170000
H	-10.61370000	7.12010000	-0.72220000
C	-9.90420000	-0.90450000	-2.42450000
H	-9.32190000	-0.28990000	-3.14680000
H	-10.97070000	-0.89220000	-2.73720000
C	-9.37870000	-2.33450000	-2.46190000
H	-8.27510000	-2.32130000	-2.33800000
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C	-7.69690000	1.54810000	-1.13090000
H	-7.08840000	2.44110000	-1.39260000
H	-7.55640000	0.81650000	-1.94760000
O	-2.69390000	-3.57490000	0.41650000
O	0.68250000	-1.04810000	1.24720000
O	-3.20200000	0.08570000	1.72660000
O	-2.66220000	2.49490000	-2.51490000
O	-1.30300000	-3.34490000	-4.11540000
O	3.15230000	-4.48250000	0.15430000
O	5.37320000	-7.34240000	0.76070000
O	6.71280000	-7.50320000	3.69570000
O	5.09410000	-4.62850000	3.45790000
O	1.34460000	4.36620000	0.29850000
O	2.46510000	7.88530000	1.98700000
O	3.09970000	10.21070000	0.05510000
O	2.47590000	7.24340000	-1.55490000
O	-6.29140000	-0.98430000	-0.86700000
O	-8.69530000	-3.38040000	1.09630000
O	-11.67230000	-2.60110000	0.32260000
O	-9.76070000	-0.39170000	-1.09370000
P	0.87270000	-3.86930000	-1.21420000
P	-0.52820000	2.43980000	0.46420000
P	-4.41450000	-1.19600000	-2.85610000
Ir	0.54840000	0.03730000	-2.71260000
Ir	-0.71240000	-2.08630000	-1.34520000
Ir	-1.28790000	0.46800000	-0.61300000
Ir	-2.14980000	-0.51120000	-3.17070000
C	1.02340000	-0.94290000	-4.29150000
O	1.29670000	-1.46370000	-5.28770000
C	2.16050000	0.09380000	-1.66380000
O	3.17200000	0.14670000	-1.10290000
C	0.43110000	1.79420000	-3.47300000
O	0.38100000	2.83030000	-3.98530000
C	-2.31200000	-0.63440000	-5.37220000

H	-1.38930000	-1.04370000	-5.76880000
H	-3.20560000	-1.13520000	-5.72590000
C	-2.39310000	0.71890000	-4.98800000
H	-3.33580000	1.25090000	-5.02540000
H	-1.52750000	1.36220000	-5.08380000

Ethyl bound at the Apical 1 position on the Tetrairidium-Calixarene complex
0 2

C	2.16490000	0.30160000	-1.85300000
C	0.23000000	1.94920000	-3.52150000
C	-1.83420000	-3.09510000	-0.47880000
C	0.02980000	-0.95830000	0.36620000
C	-2.56430000	0.06450000	1.03860000
C	-2.43440000	1.48120000	-1.95170000
C	-2.43380000	0.25730000	-4.75320000
C	-1.11680000	-2.16850000	-3.39560000
C	0.31930000	-5.31940000	-1.06710000
C	0.59420000	-6.08380000	0.08440000
H	1.32330000	-5.75620000	0.80710000
C	-0.07560000	-7.22260000	0.33380000
H	0.13250000	-7.78110000	1.23610000
C	-1.06050000	-7.68360000	-0.54650000
H	-1.59190000	-8.60200000	-0.33320000
C	-1.37350000	-6.94400000	-1.68770000
H	-2.14850000	-7.28400000	-2.36170000
C	-0.69490000	-5.75070000	-1.93960000
H	-0.97100000	-5.15770000	-2.80120000
C	2.15410000	-3.81280000	-2.84190000
C	1.99010000	-4.84380000	-3.78430000
H	1.23770000	-5.60390000	-3.66230000
C	2.81530000	-4.91090000	-4.91180000
H	2.68010000	-5.70610000	-5.63340000
C	3.82340000	-3.96380000	-5.10150000
H	4.46780000	-4.02370000	-5.96890000
C	4.00710000	-2.94690000	-4.16430000
H	4.79710000	-2.21990000	-4.30200000
C	3.17400000	-2.86860000	-3.04500000
H	3.34470000	-2.08160000	-2.32890000
C	2.26680000	-3.38570000	0.03420000
H	2.64930000	-2.35260000	-0.10170000
H	1.70030000	-3.42260000	0.98620000
C	4.61190000	-3.90900000	-0.19920000
C	5.33250000	-4.56050000	-1.21950000
C	6.50370000	-3.97960000	-1.71990000
H	6.98480000	-4.44120000	-2.57060000
C	7.07870000	-2.84650000	-1.12770000

C	6.42180000	-2.28210000	-0.01580000
H	6.83180000	-1.41770000	0.48330000
C	5.21360000	-2.80950000	0.47670000
C	8.40300000	-2.29650000	-1.69400000
C	8.15110000	-1.73870000	-3.11030000
H	7.78030000	-2.52950000	-3.79660000
H	9.08860000	-1.32570000	-3.54200000
H	7.39190000	-0.92720000	-3.07720000
C	9.44960000	-3.43480000	-1.76960000
H	9.22180000	-4.14710000	-2.58910000
H	9.46610000	-4.00830000	-0.81940000
H	10.46850000	-3.03580000	-1.96430000
C	9.00060000	-1.15960000	-0.83280000
H	9.97660000	-0.82030000	-1.24250000
H	9.16660000	-1.49700000	0.21220000
H	8.32460000	-0.28180000	-0.82760000
C	4.88820000	-5.88750000	-1.79800000
H	3.95440000	-6.25830000	-1.33070000
H	4.65980000	-5.73980000	-2.87320000
C	5.99950000	-6.90630000	-1.63130000
C	6.33640000	-7.40840000	-0.35850000
C	7.55830000	-8.08550000	-0.17290000
C	8.36670000	-8.37260000	-1.28350000
H	9.29010000	-8.90290000	-1.10660000
C	8.00320000	-7.95980000	-2.58420000
C	6.81370000	-7.21710000	-2.73070000
H	6.53990000	-6.82660000	-3.70160000
C	8.88150000	-8.23750000	-3.82280000
C	8.05450000	-8.99910000	-4.88220000
H	7.20070000	-8.39300000	-5.25010000
H	7.65410000	-9.94330000	-4.45350000
H	8.68140000	-9.25420000	-5.76420000
C	9.36920000	-6.89790000	-4.41630000
H	8.52180000	-6.26610000	-4.75510000
H	10.02730000	-7.07300000	-5.29490000
H	9.94680000	-6.32820000	-3.65660000
C	10.13200000	-9.09270000	-3.50430000
H	9.83970000	-10.07490000	-3.07360000
H	10.80550000	-8.56450000	-2.79500000
H	10.71850000	-9.29260000	-4.42740000
C	4.50810000	-8.25420000	0.73240000
H	4.98300000	-9.25620000	0.83770000
H	3.88270000	-8.25850000	-0.18790000
C	3.61140000	-8.00180000	1.93660000
H	4.24050000	-7.91950000	2.84350000
H	3.06760000	-7.04620000	1.79580000

C	2.60820000	-9.13430000	2.13130000
H	1.92390000	-8.88370000	2.96910000
H	3.13610000	-10.08030000	2.37480000
H	2.01000000	-9.28540000	1.20850000
C	8.03000000	-8.47310000	1.21210000
H	8.84600000	-9.22630000	1.15630000
H	7.20430000	-8.97390000	1.75420000
C	8.55020000	-7.26130000	1.95560000
C	7.89700000	-6.76340000	3.10120000
C	8.36840000	-5.58460000	3.71510000
C	9.57730000	-5.01940000	3.28310000
H	9.96470000	-4.16640000	3.82200000
C	10.29050000	-5.54060000	2.18750000
C	9.73320000	-6.64700000	1.50930000
H	10.22390000	-7.07650000	0.64900000
C	11.65950000	-4.93040000	1.81280000
C	11.53650000	-3.39980000	1.62550000
H	12.49050000	-2.96770000	1.25310000
H	11.29940000	-2.88060000	2.57680000
H	10.74100000	-3.16150000	0.89520000
C	12.65990000	-5.21660000	2.95150000
H	13.66420000	-4.80760000	2.70620000
H	12.75810000	-6.31180000	3.11460000
H	12.32830000	-4.75280000	3.90490000
C	12.24520000	-5.51660000	0.50510000
H	13.20790000	-5.02390000	0.24740000
H	11.54730000	-5.35990000	-0.34510000
H	12.45450000	-6.60280000	0.61260000
C	7.17480000	-8.30450000	4.72670000
H	7.54980000	-7.69040000	5.57430000
H	7.98910000	-9.00120000	4.42250000
C	5.96640000	-9.10760000	5.20940000
H	6.17830000	-9.50850000	6.22420000
H	5.07890000	-8.44390000	5.28350000
C	5.65830000	-10.28010000	4.28150000
H	4.73270000	-10.79060000	4.62140000
H	6.49400000	-11.01150000	4.29770000
H	5.50980000	-9.92950000	3.24150000
C	7.59730000	-4.88680000	4.81320000
H	6.74120000	-5.49030000	5.17960000
H	8.26700000	-4.74980000	5.69030000
C	7.08980000	-3.55320000	4.30540000
C	5.91100000	-3.48120000	3.53730000
C	5.57830000	-2.25080000	2.89930000
C	6.31350000	-1.09650000	3.22050000
H	6.05460000	-0.16650000	2.73230000

C	7.42110000	-1.13390000	4.08960000
C	7.80790000	-2.38680000	4.60460000
H	8.68500000	-2.48490000	5.22580000
C	8.21680000	0.15990000	4.36610000
C	8.87350000	0.63880000	3.05500000
H	9.45730000	1.56990000	3.22190000
H	8.11360000	0.85130000	2.27870000
H	9.55970000	-0.14070000	2.65790000
C	9.34070000	-0.02720000	5.41420000
H	9.85040000	0.93880000	5.62220000
H	10.11760000	-0.73220000	5.04680000
H	8.92530000	-0.40390000	6.37390000
C	7.26590000	1.25640000	4.89960000
H	7.83060000	2.18170000	5.14560000
H	6.75100000	0.90620000	5.82020000
H	6.49320000	1.53520000	4.15410000
C	3.77310000	-4.50400000	3.61880000
H	3.26500000	-4.77720000	2.67210000
H	3.44340000	-3.49250000	3.94930000
C	3.35520000	-5.47890000	4.71870000
H	3.73740000	-5.11390000	5.69670000
H	3.80120000	-6.47470000	4.53260000
C	1.83740000	-5.61900000	4.78910000
H	1.56660000	-6.31830000	5.60790000
H	1.44290000	-6.02400000	3.83230000
H	1.36780000	-4.63290000	4.99190000
C	4.62130000	-2.16370000	1.71870000
H	4.40930000	-1.10110000	1.46750000
H	3.64250000	-2.56710000	1.99240000
C	-2.00320000	3.54650000	1.21840000
C	-3.29310000	3.28580000	0.92060000
H	-3.57210000	2.39810000	0.37670000
C	-4.30690000	4.17760000	1.30710000
H	-5.33660000	3.95710000	1.05610000
C	-4.00780000	5.30000000	1.98810000
H	-4.80130000	5.97480000	2.28380000
C	-2.73270000	5.58990000	2.30530000
H	-2.50250000	6.49300000	2.85610000
C	-1.70000000	4.72210000	1.92510000
H	-0.68420000	4.95750000	2.19300000
C	0.33850000	2.03960000	2.16810000
C	-0.20830000	2.12560000	3.45780000
H	-1.23700000	2.42610000	3.60400000
C	0.57000000	1.80300000	4.57450000
H	0.14530000	1.87460000	5.56740000
C	1.89140000	1.37700000	4.41080000

H	2.49090000	1.12520000	5.27590000
C	2.43700000	1.27190000	3.12930000
H	3.45890000	0.93860000	3.00090000
C	1.66410000	1.60210000	2.01260000
H	2.09800000	1.50680000	1.02670000
C	0.40710000	3.43680000	-0.37880000
H	1.03250000	2.72160000	-0.94800000
H	-0.24350000	4.00780000	-1.07210000
C	2.50960000	4.35820000	0.30880000
C	3.26640000	4.58560000	1.48320000
C	4.64950000	4.33700000	1.47920000
H	5.18170000	4.44750000	2.41040000
C	5.32280000	3.92020000	0.31730000
C	4.57630000	3.80120000	-0.86220000
H	5.07530000	3.53530000	-1.78440000
C	3.21080000	4.11140000	-0.90880000
C	6.83930000	3.65600000	0.27530000
C	7.49120000	4.58820000	-0.77280000
H	7.15220000	5.63460000	-0.62020000
H	7.21980000	4.29580000	-1.80860000
H	8.60010000	4.55530000	-0.70500000
C	7.53590000	3.90250000	1.63610000
H	7.13580000	3.21900000	2.41450000
H	7.39330000	4.95170000	1.97050000
H	8.62940000	3.71750000	1.56150000
C	7.08750000	2.18810000	-0.12410000
H	6.56080000	1.50160000	0.57350000
H	8.17490000	1.96100000	-0.09840000
H	6.72330000	1.97560000	-1.15140000
C	2.61390000	4.94290000	2.80690000
H	1.52320000	5.04230000	2.73980000
H	2.73600000	4.05930000	3.46710000
C	3.27450000	6.16220000	3.44460000
C	3.26020000	7.46870000	2.86400000
C	4.27810000	8.37900000	3.22140000
C	5.18170000	8.06780000	4.24650000
H	5.93330000	8.80280000	4.49170000
C	5.12770000	6.83450000	4.92220000
C	4.15800000	5.90370000	4.50870000
H	4.14990000	4.92140000	4.96140000
C	6.13490000	6.44070000	6.02440000
C	5.37090000	6.07720000	7.31670000
H	4.71760000	5.19170000	7.17210000
H	4.73660000	6.92980000	7.64260000
H	6.07890000	5.83390000	8.13850000
C	7.13070000	7.57330000	6.37340000

H	7.75970000	7.83440000	5.49480000
H	7.81800000	7.25690000	7.18800000
H	6.59120000	8.47980000	6.72360000
C	6.95960000	5.22120000	5.55390000
H	7.48060000	5.45200000	4.59950000
H	6.31890000	4.32970000	5.39170000
H	7.72470000	4.94580000	6.31170000
C	1.00860000	7.45210000	2.06300000
H	0.75230000	7.06400000	3.07460000
H	0.84180000	6.67570000	1.29630000
C	0.06160000	8.61230000	1.75790000
H	0.35860000	9.09670000	0.80610000
H	-0.96960000	8.21700000	1.63390000
C	0.06000000	9.65430000	2.87340000
H	-0.64030000	10.47520000	2.61190000
H	1.07390000	10.08460000	3.00610000
H	-0.27170000	9.19610000	3.82930000
C	4.41070000	9.70460000	2.50200000
H	3.40850000	10.16550000	2.39630000
H	5.00900000	10.42840000	3.09780000
C	5.08830000	9.49040000	1.16930000
C	4.38210000	9.57770000	-0.04730000
C	5.00520000	9.17130000	-1.24340000
C	6.36960000	8.82990000	-1.23190000
H	6.82770000	8.57530000	-2.17550000
C	7.13180000	8.87520000	-0.04300000
C	6.45490000	9.17690000	1.15420000
H	6.99380000	9.19960000	2.09110000
C	8.66670000	8.69430000	-0.02620000
C	9.31930000	10.04840000	0.32010000
H	9.02800000	10.82070000	-0.42460000
H	10.42780000	9.96370000	0.32090000
H	9.00440000	10.40050000	1.32560000
C	9.23520000	8.22550000	-1.38800000
H	9.06640000	8.98990000	-2.17680000
H	8.76930000	7.26670000	-1.70120000
H	10.33300000	8.06280000	-1.32340000
C	9.08490000	7.65250000	1.03760000
H	8.56100000	6.69440000	0.86990000
H	8.86300000	7.99500000	2.06890000
H	10.17860000	7.45900000	0.99290000
C	3.07350000	11.53220000	-0.10560000
H	3.63660000	11.90820000	-0.98990000
H	3.56630000	11.93350000	0.80720000
C	1.63690000	12.05730000	-0.14120000
H	1.63240000	13.11940000	0.18670000

H	1.00740000	11.48080000	0.56900000
C	1.03440000	11.98610000	-1.54220000
H	-0.01850000	12.33710000	-1.51140000
H	1.04920000	10.94880000	-1.92760000
H	1.60440000	12.63720000	-2.23860000
C	4.25550000	9.15620000	-2.55810000
H	4.79010000	9.82910000	-3.26350000
H	3.24120000	9.58810000	-2.46950000
C	4.17370000	7.75030000	-3.11870000
C	3.30820000	6.77800000	-2.56630000
C	3.39430000	5.44240000	-2.99860000
C	4.26420000	5.10240000	-4.04270000
H	4.31210000	4.06880000	-4.35810000
C	5.10250000	6.06050000	-4.64510000
C	5.04060000	7.38660000	-4.16340000
H	5.68850000	8.15070000	-4.56510000
C	6.08070000	5.61950000	-5.75470000
C	6.92090000	6.78700000	-6.32680000
H	7.59490000	6.42870000	-7.13510000
H	7.56220000	7.23870000	-5.53900000
H	6.26380000	7.57080000	-6.76210000
C	5.28790000	4.99780000	-6.92560000
H	5.96900000	4.71640000	-7.75800000
H	4.54180000	5.72400000	-7.31490000
H	4.75030000	4.07790000	-6.61490000
C	7.06270000	4.57220000	-5.18470000
H	7.80300000	4.26570000	-5.95520000
H	6.53500000	3.65550000	-4.84760000
H	7.61570000	4.99400000	-4.31750000
C	1.26020000	7.86130000	-1.98520000
H	1.34300000	8.19530000	-3.04590000
H	1.19860000	8.76150000	-1.34750000
C	-0.02440000	7.04640000	-1.82650000
H	-0.05110000	6.56910000	-0.82650000
H	-0.05420000	6.25000000	-2.59910000
C	-1.26210000	7.92370000	-1.98640000
H	-2.17470000	7.29990000	-1.88120000
H	-1.26920000	8.40080000	-2.98950000
H	-1.28120000	8.71280000	-1.20490000
C	2.62150000	4.35360000	-2.28590000
H	2.66010000	3.40040000	-2.85590000
H	1.56970000	4.67260000	-2.25360000
C	-5.61230000	-0.36610000	-3.77760000
C	-5.65580000	1.03550000	-3.78040000
H	-5.00360000	1.60320000	-3.13530000
C	-6.55930000	1.71610000	-4.60070000

H	-6.59230000	2.79780000	-4.58800000
C	-7.41820000	1.00110000	-5.43700000
H	-8.11440000	1.52790000	-6.07640000
C	-7.37870000	-0.39470000	-5.44690000
H	-8.04150000	-0.94530000	-6.10090000
C	-6.48910000	-1.07970000	-4.61190000
H	-6.49670000	-2.15960000	-4.62320000
C	-4.47690000	-2.99240000	-3.07670000
C	-4.09370000	-3.45840000	-4.34170000
H	-3.79760000	-2.76330000	-5.11740000
C	-4.08160000	-4.83530000	-4.60070000
H	-3.78440000	-5.19280000	-5.57830000
C	-4.42340000	-5.71560000	-3.64120000
H	-4.39700000	-6.77620000	-3.85810000
C	-4.78940000	-5.30060000	-2.41390000
H	-5.04210000	-6.02840000	-1.65440000
C	-4.83620000	-3.93480000	-2.10470000
H	-5.12150000	-3.63280000	-1.11260000
C	-4.93820000	-0.89940000	-0.99680000
H	-4.35740000	-1.54520000	-0.30920000
H	-4.67670000	0.16210000	-0.78990000
C	-6.78780000	-0.45720000	0.35260000
C	-6.51710000	-0.99660000	1.62920000
C	-6.59540000	-0.16570000	2.75690000
H	-6.30040000	-0.56800000	3.71530000
C	-7.02990000	1.16810000	2.66850000
C	-7.42190000	1.64680000	1.40210000
H	-7.78750000	2.65500000	1.27830000
C	-7.31430000	0.84770000	0.25190000
C	-7.05440000	2.04010000	3.94080000
C	-5.61100000	2.22330000	4.45700000
H	-4.97750000	2.69910000	3.67890000
H	-5.14930000	1.25020000	4.72750000
H	-5.59580000	2.86750000	5.36280000
C	-7.89920000	1.34250000	5.03170000
H	-8.87690000	1.02340000	4.61790000
H	-8.08100000	2.01950000	5.89430000
H	-7.38810000	0.44160000	5.42850000
C	-7.65420000	3.44700000	3.70130000
H	-8.69480000	3.37440000	3.31990000
H	-7.03960000	4.02400000	2.97760000
H	-7.68140000	4.03110000	4.64670000
C	-6.13700000	-2.44720000	1.82840000
H	-6.00970000	-2.96640000	0.87010000
H	-5.13160000	-2.47870000	2.30200000
C	-7.17080000	-3.13260000	2.71270000

C	-8.49550000	-3.39380000	2.26100000
C	-9.53360000	-3.48250000	3.20850000
C	-9.22910000	-3.53720000	4.57470000
H	-10.04090000	-3.65680000	5.27940000
C	-7.90490000	-3.44180000	5.04070000
C	-6.88750000	-3.22480000	4.08740000
H	-5.87110000	-3.04290000	4.40210000
C	-7.62820000	-3.51810000	6.55780000
C	-8.39180000	-2.38750000	7.28330000
H	-9.49080000	-2.49630000	7.17440000
H	-8.09850000	-1.39820000	6.87330000
H	-8.16540000	-2.39450000	8.37170000
C	-8.10500000	-4.88480000	7.09580000
H	-9.20010000	-5.01460000	6.96870000
H	-7.88280000	-4.98140000	8.18080000
H	-7.59130000	-5.71150000	6.55880000
C	-6.12850000	-3.37240000	6.91220000
H	-5.52740000	-4.17150000	6.42660000
H	-5.97250000	-3.45760000	8.00970000
H	-5.74190000	-2.37800000	6.59980000
C	-7.99150000	-4.40720000	0.17950000
H	-7.16810000	-4.88650000	0.75740000
H	-7.55870000	-3.81360000	-0.65050000
C	-8.85360000	-5.53220000	-0.39380000
H	-9.24020000	-6.15860000	0.43910000
H	-9.72140000	-5.10470000	-0.93160000
C	-8.06520000	-6.41010000	-1.35870000
H	-8.72480000	-7.21010000	-1.75560000
H	-7.20920000	-6.88490000	-0.83450000
H	-7.69230000	-5.80440000	-2.21190000
C	-10.97950000	-3.57220000	2.76970000
H	-11.06220000	-4.26140000	1.90340000
H	-11.60550000	-4.02930000	3.56700000
C	-11.52500000	-2.19420000	2.46280000
C	-11.87600000	-1.81380000	1.15170000
C	-12.32190000	-0.50030000	0.90070000
C	-12.53170000	0.37470000	1.97580000
H	-12.93100000	1.35760000	1.76640000
C	-12.22980000	0.00740000	3.30010000
C	-11.70420000	-1.28460000	3.51960000
H	-11.44710000	-1.61760000	4.51360000
C	-12.50540000	1.00690000	4.44400000
C	-11.80650000	2.35510000	4.14910000
H	-12.26690000	2.87990000	3.28650000
H	-10.73540000	2.19350000	3.91870000
H	-11.87910000	3.04130000	5.02040000

C	-14.02660000	1.24050000	4.55190000
H	-14.43650000	1.67440000	3.61520000
H	-14.25920000	1.94380000	5.38080000
H	-14.55240000	0.28100000	4.74850000
C	-12.00280000	0.50640000	5.82030000
H	-12.18580000	1.26840000	6.60880000
H	-10.91080000	0.30430000	5.79370000
H	-12.53840000	-0.41740000	6.12840000
C	-12.99530000	-3.40640000	-0.17100000
H	-13.79200000	-2.66940000	-0.41810000
H	-13.31350000	-3.99220000	0.72050000
C	-12.80560000	-4.35220000	-1.35360000
H	-12.06130000	-5.13090000	-1.08670000
H	-12.42510000	-3.77980000	-2.22650000
C	-14.11610000	-5.03300000	-1.73580000
H	-13.94200000	-5.71890000	-2.59150000
H	-14.87140000	-4.27570000	-2.03600000
H	-14.50770000	-5.62380000	-0.88040000
C	-12.54840000	0.01440000	-0.50360000
H	-12.49280000	-0.79140000	-1.25900000
H	-13.58290000	0.41640000	-0.57000000
C	-11.52960000	1.08870000	-0.81950000
C	-10.17900000	0.76140000	-1.05560000
C	-9.20480000	1.77700000	-1.05870000
C	-9.59880000	3.12010000	-0.96620000
H	-8.82360000	3.87110000	-0.98120000
C	-10.95590000	3.47690000	-0.80710000
C	-11.90580000	2.43710000	-0.73170000
H	-12.94640000	2.67110000	-0.55160000
C	-11.41900000	4.94010000	-0.64490000
C	-12.06060000	5.12210000	0.74850000
H	-12.36150000	6.18010000	0.90880000
H	-11.33900000	4.83900000	1.54550000
H	-12.97010000	4.49660000	0.86620000
C	-12.45660000	5.27770000	-1.73810000
H	-12.02320000	5.10690000	-2.74730000
H	-12.77140000	6.34160000	-1.66840000
H	-13.37110000	4.65640000	-1.64150000
C	-10.26300000	5.96260000	-0.76640000
H	-9.76420000	5.87960000	-1.75640000
H	-9.51190000	5.81150000	0.03900000
H	-10.64460000	7.00240000	-0.67000000
C	-9.89640000	-0.98370000	-2.52840000
H	-9.27910000	-0.35830000	-3.21140000
H	-10.94870000	-0.95450000	-2.88510000
C	-9.38170000	-2.41730000	-2.57570000

H	-8.28260000	-2.41580000	-2.41590000
H	-9.86140000	-2.99320000	-1.76150000
C	-9.69540000	-3.09600000	-3.90440000
H	-9.28990000	-4.12970000	-3.89560000
H	-9.23240000	-2.54030000	-4.74350000
H	-10.79310000	-3.14670000	-4.06370000
C	-7.73400000	1.42760000	-1.07950000
H	-7.11030000	2.32420000	-1.28740000
H	-7.55520000	0.71710000	-1.90760000
O	3.17720000	0.42590000	-1.29770000
O	0.08870000	2.99410000	-3.99870000
O	-2.60130000	-3.73970000	0.10450000
O	0.70680000	-1.08340000	1.32260000
O	-3.21090000	-0.17570000	1.97200000
O	-2.82440000	2.57470000	-2.15050000
O	-2.58490000	0.62380000	-5.84350000
O	-0.92820000	-2.88130000	-4.31660000
O	3.31110000	-4.36810000	0.08270000
O	5.51510000	-7.23590000	0.66530000
O	6.80210000	-7.45650000	3.63460000
O	5.19130000	-4.59720000	3.42500000
O	1.17810000	4.34020000	0.42910000
O	2.36380000	7.90140000	1.97390000
O	3.08150000	10.10030000	-0.07720000
O	2.39470000	7.10080000	-1.55040000
O	-6.34240000	-1.10990000	-0.81050000
O	-8.82240000	-3.55140000	0.97920000
O	-11.76420000	-2.73250000	0.10090000
O	-9.80470000	-0.50230000	-1.18150000
P	1.09490000	-3.68560000	-1.35260000
P	-0.67040000	2.40870000	0.69250000
P	-4.38770000	-1.20730000	-2.72080000
Ir	0.47890000	0.25610000	-2.70980000
Ir	-0.58500000	-1.98380000	-1.36730000
Ir	-1.39480000	0.42500000	-0.39090000
Ir	-2.15830000	-0.32940000	-3.00670000
C	1.33590000	-0.32940000	-4.64180000
C	2.64290000	0.31850000	-5.06400000
H	0.53910000	-0.11950000	-5.35750000
H	1.42450000	-1.41130000	-4.53550000
H	2.96270000	-0.08380000	-6.03710000
H	2.54770000	1.40350000	-5.17880000
H	3.45130000	0.12880000	-4.35040000

Ethyl bound at the Basal 2 position on the Tetrairidium-Calixarene complex
0 2

C	0.26280000	-1.35510000	0.39600000
C	-2.41010000	-0.31570000	0.95420000
C	-2.29170000	0.97670000	-2.00720000
C	-0.90100000	-3.33780000	-2.81160000
C	0.87790000	-5.72380000	-0.42110000
C	1.30390000	-6.25980000	0.81120000
H	2.00640000	-5.72960000	1.43350000
C	0.81350000	-7.42610000	1.26540000
H	1.13330000	-7.80420000	2.22710000
C	-0.12170000	-8.15030000	0.51880000
H	-0.50770000	-9.08840000	0.89610000
C	-0.56740000	-7.65300000	-0.70650000
H	-1.30070000	-8.20100000	-1.28390000
C	-0.07380000	-6.43370000	-1.17310000
H	-0.44240000	-6.04150000	-2.10970000
C	2.37860000	-4.28840000	-2.54160000
C	2.36080000	-5.49260000	-3.26870000
H	1.82440000	-6.35700000	-2.91700000
C	3.05820000	-5.59990000	-4.47680000
H	3.03500000	-6.52790000	-5.03330000
C	3.80280000	-4.51990000	-4.95560000
H	4.35220000	-4.60920000	-5.88370000
C	3.84990000	-3.33020000	-4.22740000
H	4.43590000	-2.49590000	-4.59070000
C	3.13510000	-3.21300000	-3.03230000
H	3.18200000	-2.28380000	-2.48650000
C	2.68600000	-3.46100000	0.20960000
H	2.92740000	-2.41740000	-0.08480000
H	2.22120000	-3.43840000	1.21490000
C	5.05440000	-3.71110000	-0.15510000
C	5.78150000	-4.32660000	-1.19320000
C	6.81940000	-3.62690000	-1.82150000
H	7.29200000	-4.07290000	-2.68520000
C	7.26980000	-2.38680000	-1.34570000
C	6.63550000	-1.85260000	-0.20630000
H	6.95960000	-0.91230000	0.21190000
C	5.55300000	-2.50470000	0.41270000
C	8.43290000	-1.68000000	-2.07140000
C	7.95930000	-1.24910000	-3.47490000
H	7.64570000	-2.12500000	-4.08210000
H	8.77530000	-0.72960000	-4.02260000
H	7.09310000	-0.55670000	-3.39550000
C	9.63050000	-2.65090000	-2.21170000
H	9.43560000	-3.43570000	-2.97160000

H	9.83200000	-3.15830000	-1.24630000
H	10.55020000	-2.11510000	-2.53190000
C	8.93030000	-0.41790000	-1.32770000
H	9.79450000	0.04040000	-1.85560000
H	9.25450000	-0.66770000	-0.29530000
H	8.13110000	0.34970000	-1.28260000
C	5.48260000	-5.73420000	-1.66050000
H	4.63210000	-6.18700000	-1.11350000
H	5.17990000	-5.68710000	-2.72440000
C	6.72210000	-6.59450000	-1.51430000
C	7.18160000	-6.99540000	-0.24470000
C	8.47850000	-7.52950000	-0.10530000
C	9.25300000	-7.77710000	-1.24930000
H	10.23800000	-8.19460000	-1.10620000
C	8.77840000	-7.46110000	-2.54100000
C	7.50660000	-6.86240000	-2.64640000
H	7.13810000	-6.55090000	-3.61450000
C	9.61750000	-7.68810000	-3.81650000
C	8.83140000	-8.58310000	-4.80000000
H	7.89420000	-8.09530000	-5.13990000
H	8.56730000	-9.54850000	-4.31640000
H	9.43700000	-8.80060000	-5.70650000
C	9.91380000	-6.32710000	-4.48350000
H	8.98200000	-5.81400000	-4.80100000
H	10.54560000	-6.46100000	-5.38820000
H	10.45410000	-5.66140000	-3.77610000
C	10.97430000	-8.37990000	-3.53880000
H	10.82170000	-9.37080000	-3.05880000
H	11.61650000	-7.74900000	-2.88670000
H	11.53200000	-8.54840000	-4.48570000
C	5.53050000	-7.97590000	1.00610000
H	6.12370000	-8.90940000	1.13610000
H	4.85870000	-8.10850000	0.12910000
C	4.68040000	-7.75060000	2.24900000
H	5.34670000	-7.55100000	3.11000000
H	4.02960000	-6.86650000	2.09340000
C	3.81740000	-8.96850000	2.56230000
H	3.19130000	-8.75880000	3.45490000
H	4.45610000	-9.85090000	2.77790000
H	3.15470000	-9.20410000	1.70300000
C	9.06960000	-7.78840000	1.26360000
H	9.96550000	-8.44290000	1.19140000
H	8.34120000	-8.35190000	1.87880000
C	9.48260000	-6.48610000	1.91460000
C	8.84180000	-6.00660000	3.07470000
C	9.19880000	-4.74680000	3.59740000

C	10.29740000	-4.06310000	3.05590000
H	10.60750000	-3.13920000	3.52220000
C	10.99010000	-4.54500000	1.93030000
C	10.54400000	-5.75430000	1.35440000
H	11.02770000	-6.16570000	0.48130000
C	12.21190000	-3.76330000	1.39990000
C	11.83630000	-2.28140000	1.15870000
H	12.66150000	-1.73870000	0.64890000
H	11.63750000	-1.74280000	2.10830000
H	10.92960000	-2.20910000	0.52820000
C	13.34140000	-3.83110000	2.44800000
H	14.24370000	-3.28920000	2.09010000
H	13.62290000	-4.88810000	2.64600000
H	13.02750000	-3.37060000	3.40890000
C	12.76120000	-4.33120000	0.06850000
H	13.60980000	-3.71680000	-0.30330000
H	11.97410000	-4.33050000	-0.71570000
H	13.14370000	-5.36600000	0.20300000
C	8.39080000	-7.52180000	4.81900000
H	8.73550000	-6.81870000	5.60830000
H	9.26300000	-8.14010000	4.50610000
C	7.30890000	-8.42370000	5.41410000
H	7.61930000	-8.73950000	6.43360000
H	6.35750000	-7.85780000	5.50680000
C	7.08560000	-9.67430000	4.56740000
H	6.24340000	-10.26300000	4.98790000
H	7.99830000	-10.30730000	4.57050000
H	6.84230000	-9.40230000	3.52170000
C	8.40610000	-4.08090000	4.70000000
H	7.64230000	-4.75490000	5.13990000
H	9.09640000	-3.82260000	5.53260000
C	7.72970000	-2.84030000	4.15400000
C	6.50480000	-2.93460000	3.46340000
C	6.01110000	-1.78680000	2.77550000
C	6.65420000	-0.55090000	2.96440000
H	6.27840000	0.31330000	2.43330000
C	7.81860000	-0.42540000	3.74600000
C	8.34870000	-1.59440000	4.32440000
H	9.26760000	-1.56610000	4.88980000
C	8.52020000	0.94530000	3.85370000
C	9.02970000	1.36230000	2.45820000
H	9.54440000	2.34650000	2.50260000
H	8.19640000	1.44910000	1.73420000
H	9.74660000	0.60820000	2.06650000
C	9.73510000	0.93650000	4.81350000
H	10.17720000	1.95310000	4.89900000

H	10.53660000	0.26370000	4.43850000
H	9.42970000	0.61420000	5.83250000
C	7.52440000	2.00380000	4.37920000
H	8.02820000	2.98670000	4.50130000
H	7.11640000	1.69480000	5.36580000
H	6.67380000	2.15650000	3.68350000
C	4.49440000	-4.16300000	3.74150000
H	3.96390000	-4.53930000	2.84410000
H	4.08120000	-3.17270000	4.04160000
C	4.24450000	-5.11480000	4.91030000
H	4.64330000	-4.66180000	5.84380000
H	4.77890000	-6.07010000	4.74300000
C	2.75570000	-5.40240000	5.08310000
H	2.60630000	-6.07770000	5.95160000
H	2.35120000	-5.89890000	4.17500000
H	2.19870000	-4.45860000	5.26460000
C	4.97370000	-1.86750000	1.66420000
H	4.62450000	-0.84990000	1.38320000
H	4.06670000	-2.35970000	2.02240000
C	-1.94940000	3.09490000	1.25010000
C	-3.22010000	2.83340000	0.87960000
H	-3.45220000	2.00730000	0.22890000
C	-4.27480000	3.64420000	1.33040000
H	-5.28900000	3.42380000	1.02210000
C	-4.03460000	4.68870000	2.14520000
H	-4.85900000	5.30050000	2.48970000
C	-2.78120000	4.97420000	2.54130000
H	-2.59940000	5.80960000	3.20520000
C	-1.70880000	4.18820000	2.09860000
H	-0.71120000	4.41770000	2.43070000
C	0.51200000	1.74130000	2.07520000
C	-0.04320000	1.58090000	3.35410000
H	-1.10940000	1.68180000	3.50870000
C	0.77720000	1.27350000	4.44430000
H	0.34490000	1.15770000	5.42970000
C	2.15260000	1.10430000	4.26200000
H	2.78590000	0.86410000	5.10610000
C	2.70870000	1.23600000	2.98780000
H	3.77270000	1.10030000	2.84520000
C	1.89160000	1.54810000	1.89750000
H	2.33680000	1.63290000	0.91720000
C	0.37910000	3.23040000	-0.43570000
H	1.07070000	2.61140000	-1.04110000
H	-0.35680000	3.73390000	-1.09450000
C	2.36380000	4.43010000	0.17040000
C	3.16200000	4.72080000	1.30390000

C	4.56300000	4.67920000	1.19850000
H	5.13830000	4.82870000	2.09860000
C	5.20470000	4.40760000	-0.02340000
C	4.40100000	4.24180000	-1.15900000
H	4.86660000	4.09380000	-2.12420000
C	3.00510000	4.34830000	-1.10160000
C	6.73640000	4.33670000	-0.17200000
C	7.19980000	5.38490000	-1.21070000
H	6.73520000	6.37000000	-0.99610000
H	6.90970000	5.09710000	-2.24280000
H	8.30540000	5.49880000	-1.20210000
C	7.48730000	4.60890000	1.15420000
H	7.22380000	3.84950000	1.91980000
H	7.24410000	5.61800000	1.54890000
H	8.58770000	4.56120000	1.00420000
C	7.13050000	2.92700000	-0.65830000
H	6.72050000	2.15460000	0.02720000
H	8.23620000	2.81910000	-0.69840000
H	6.73600000	2.72090000	-1.67560000
C	2.56190000	4.91960000	2.68420000
H	1.46790000	4.85100000	2.69110000
H	2.86630000	4.04080000	3.29070000
C	3.06530000	6.20340000	3.33880000
C	2.80040000	7.51240000	2.82960000
C	3.66830000	8.56680000	3.18580000
C	4.66440000	8.37070000	4.15140000
H	5.29220000	9.21250000	4.40150000
C	4.85570000	7.11790000	4.76330000
C	4.03940000	6.05210000	4.34260000
H	4.22010000	5.06420000	4.74390000
C	5.96620000	6.85820000	5.80400000
C	5.33640000	6.31930000	7.10720000
H	4.83260000	5.34340000	6.94660000
H	4.58580000	7.03930000	7.49950000
H	6.11370000	6.16500000	7.88680000
C	6.77370000	8.12840000	6.16550000
H	7.30580000	8.52800000	5.27500000
H	7.54360000	7.90060000	6.93460000
H	6.10770000	8.91510000	6.58160000
C	6.95950000	5.81620000	5.24360000
H	7.38430000	6.16630000	4.27770000
H	6.46820000	4.83670000	5.07130000
H	7.79750000	5.64650000	5.95400000
C	0.53270000	7.17570000	2.16510000
H	0.41230000	6.71040000	3.16960000
H	0.42030000	6.41380000	1.37480000

C	-0.58900000	8.19920000	1.98620000
H	-0.41430000	8.78810000	1.06360000
H	-1.55630000	7.66570000	1.87060000
C	-0.68850000	9.14830000	3.17730000
H	-1.50750000	9.87720000	3.00250000
H	0.26000000	9.70790000	3.31020000
H	-0.91170000	8.58040000	4.10550000
C	3.53470000	9.92590000	2.53210000
H	2.46650000	10.22010000	2.51640000
H	4.05230000	10.71210000	3.12440000
C	4.13840000	9.88110000	1.14880000
C	3.34040000	9.91150000	-0.01230000
C	3.92890000	9.65790000	-1.26640000
C	5.32640000	9.52930000	-1.36220000
H	5.74820000	9.38900000	-2.34560000
C	6.15710000	9.63360000	-0.22420000
C	5.53160000	9.77990000	1.02840000
H	6.12730000	9.84090000	1.92860000
C	7.69940000	9.66980000	-0.31480000
C	8.18280000	11.08700000	0.05520000
H	7.73900000	11.83950000	-0.63220000
H	9.29000000	11.15740000	-0.01630000
H	7.89120000	11.35240000	1.09390000
C	8.22970000	9.33940000	-1.73160000
H	7.90390000	10.10400000	-2.46930000
H	7.87770000	8.33860000	-2.06140000
H	9.34120000	9.32880000	-1.74540000
C	8.32850000	8.65470000	0.66830000
H	7.91250000	7.64430000	0.50240000
H	8.15060000	8.93350000	1.72710000
H	9.43040000	8.60180000	0.53250000
C	1.75150000	11.64090000	0.12420000
H	2.17470000	12.13680000	-0.77860000
H	2.25320000	12.07360000	1.01770000
C	0.25490000	11.93970000	0.22890000
H	0.11970000	12.98080000	0.59440000
H	-0.21440000	11.25730000	0.96850000
C	-0.45220000	11.80890000	-1.11770000
H	-1.53770000	12.00190000	-0.98680000
H	-0.32310000	10.79210000	-1.53490000
H	-0.04530000	12.54930000	-1.83880000
C	3.09580000	9.57810000	-2.52720000
H	3.46000000	10.36190000	-3.22660000
H	2.03390000	9.83010000	-2.34760000
C	3.20530000	8.20480000	-3.15960000
C	2.55460000	7.07660000	-2.60820000

C	2.83310000	5.79450000	-3.11550000
C	3.67740000	5.65240000	-4.22450000
H	3.87670000	4.65650000	-4.59660000
C	4.30100000	6.76420000	-4.82380000
C	4.04770000	8.03870000	-4.27180000
H	4.52950000	8.91850000	-4.67040000
C	5.26630000	6.54440000	-6.00820000
C	5.85970000	7.86140000	-6.56470000
H	6.53140000	7.65790000	-7.42700000
H	6.46480000	8.38280000	-5.79150000
H	5.05370000	8.53870000	-6.92150000
C	4.51600000	5.84620000	-7.16380000
H	5.18010000	5.72020000	-8.04640000
H	3.63530000	6.45000000	-7.47250000
H	4.16140000	4.83590000	-6.87180000
C	6.44510000	5.65780000	-5.54940000
H	7.17630000	5.51620000	-6.37470000
H	6.10210000	4.65070000	-5.23280000
H	6.97260000	6.13080000	-4.69270000
C	0.40180000	7.77820000	-1.84590000
H	0.35360000	8.16150000	-2.89190000
H	0.24430000	8.63150000	-1.16230000
C	-0.72170000	6.75990000	-1.64430000
H	-0.59610000	6.24150000	-0.67320000
H	-0.68400000	6.00330000	-2.45570000
C	-2.09160000	7.43060000	-1.66850000
H	-2.88260000	6.66290000	-1.53370000
H	-2.25260000	7.94310000	-2.64080000
H	-2.17430000	8.17160000	-0.84500000
C	2.29220000	4.56100000	-2.42410000
H	2.44060000	3.65560000	-3.05100000
H	1.20870000	4.70540000	-2.31480000
C	-5.57000000	-0.85360000	-3.70550000
C	-5.58270000	0.54340000	-3.83260000
H	-4.93290000	1.15300000	-3.22300000
C	-6.44700000	1.16630000	-4.73660000
H	-6.45510000	2.24520000	-4.82130000
C	-7.29700000	0.39710000	-5.53250000
H	-7.96190000	0.87870000	-6.23770000
C	-7.29000000	-0.99440000	-5.41680000
H	-7.94680000	-1.58680000	-6.03930000
C	-6.44230000	-1.62030000	-4.49610000
H	-6.47960000	-2.69560000	-4.40770000
C	-4.49790000	-3.42610000	-2.72220000
C	-4.18230000	-4.01710000	-3.95360000
H	-3.93570000	-3.40370000	-4.81120000

C	-4.16910000	-5.41340000	-4.07190000
H	-3.92820000	-5.86680000	-5.02490000
C	-4.43360000	-6.19380000	-3.00710000
H	-4.40430000	-7.27070000	-3.11580000
C	-4.72390000	-5.65810000	-1.80670000
H	-4.91360000	-6.30580000	-0.96090000
C	-4.77200000	-4.26840000	-1.63610000
H	-4.98360000	-3.87220000	-0.65940000
C	-5.00150000	-1.12670000	-0.88260000
H	-4.45430000	-1.69390000	-0.10910000
H	-4.75490000	-0.04690000	-0.77120000
C	-6.91030000	-0.60290000	0.35590000
C	-6.70830000	-1.04810000	1.68140000
C	-6.89750000	-0.15180000	2.74360000
H	-6.67680000	-0.48580000	3.74720000
C	-7.37520000	1.15320000	2.53880000
C	-7.67050000	1.54370000	1.21750000
H	-8.05750000	2.52820000	1.00320000
C	-7.46000000	0.67680000	0.13260000
C	-7.59420000	2.07360000	3.75640000
C	-6.24650000	2.31680000	4.46950000
H	-5.51490000	2.77140000	3.77050000
H	-5.81080000	1.37170000	4.85600000
H	-6.37720000	3.00300000	5.33420000
C	-8.57220000	1.39010000	4.73830000
H	-9.46580000	1.02010000	4.19540000
H	-8.90000000	2.09150000	5.53580000
H	-8.10130000	0.51950000	5.23830000
C	-8.18200000	3.45380000	3.37520000
H	-9.16600000	3.34160000	2.87220000
H	-7.48920000	4.00680000	2.70430000
H	-8.33770000	4.08040000	4.28020000
C	-6.30760000	-2.47040000	2.00630000
H	-6.12590000	-3.05530000	1.09670000
H	-5.32510000	-2.44020000	2.52590000
C	-7.36640000	-3.11520000	2.89260000
C	-8.67130000	-3.41570000	2.40950000
C	-9.74590000	-3.43700000	3.32040000
C	-9.49290000	-3.40080000	4.69790000
H	-10.33070000	-3.47460000	5.37810000
C	-8.18550000	-3.28620000	5.20610000
C	-7.13350000	-3.12370000	4.27980000
H	-6.12970000	-2.91990000	4.62030000
C	-7.96210000	-3.29160000	6.73410000
C	-8.73380000	-2.11890000	7.37860000
H	-9.82870000	-2.21000000	7.22220000

H	-8.39940000	-1.15260000	6.94640000
H	-8.55740000	-2.08760000	8.47570000
C	-8.47550000	-4.62490000	7.32010000
H	-9.56790000	-4.74610000	7.16470000
H	-8.28910000	-4.67320000	8.41500000
H	-7.95750000	-5.48290000	6.83940000
C	-6.47330000	-3.14790000	7.13290000
H	-5.86700000	-3.97500000	6.70400000
H	-6.35570000	-3.18520000	8.23790000
H	-6.06280000	-2.17330000	6.79040000
C	-8.06270000	-4.56490000	0.42610000
H	-7.25900000	-4.98990000	1.07020000
H	-7.60110000	-4.01660000	-0.41990000
C	-8.87580000	-5.74320000	-0.11070000
H	-9.28450000	-6.32600000	0.74310000
H	-9.72870000	-5.37120000	-0.70950000
C	-8.02890000	-6.66020000	-0.98570000
H	-8.65530000	-7.49580000	-1.36230000
H	-7.18940000	-7.08540000	-0.39660000
H	-7.62870000	-6.09860000	-1.85650000
C	-11.17300000	-3.57480000	2.83530000
H	-11.21590000	-4.33150000	2.02430000
H	-11.82600000	-3.97670000	3.64080000
C	-11.72140000	-2.23290000	2.39890000
C	-12.01390000	-1.96120000	1.04710000
C	-12.47410000	-0.68210000	0.67470000
C	-12.77000000	0.26110000	1.66870000
H	-13.19010000	1.20990000	1.36470000
C	-12.54400000	-0.00340000	3.03250000
C	-11.98300000	-1.25440000	3.37440000
H	-11.77410000	-1.50710000	4.40290000
C	-12.96460000	1.04420000	4.08690000
C	-12.34290000	2.42180000	3.75500000
H	-12.76490000	2.85460000	2.82460000
H	-11.24730000	2.33490000	3.62610000
H	-12.54100000	3.15330000	4.56800000
C	-14.50200000	1.17320000	4.07560000
H	-14.87070000	1.51810000	3.08620000
H	-14.84150000	1.90700000	4.83850000
H	-14.97450000	0.19200000	4.29870000
C	-12.53050000	0.66490000	5.52390000
H	-12.81480000	1.46120000	6.24570000
H	-11.42950000	0.53310000	5.58360000
H	-13.02930000	-0.27040000	5.85770000
C	-13.05280000	-3.67190000	-0.18980000
H	-13.84560000	-2.97100000	-0.53510000

H	-13.40570000	-4.18410000	0.73340000
C	-12.79850000	-4.71300000	-1.27610000
H	-12.05940000	-5.45500000	-0.90900000
H	-12.38450000	-4.21260000	-2.17720000
C	-14.08260000	-5.44340000	-1.65680000
H	-13.86170000	-6.19790000	-2.44090000
H	-14.83120000	-4.72590000	-2.05540000
H	-14.50710000	-5.96390000	-0.77190000
C	-12.63950000	-0.28160000	-0.77450000
H	-12.53920000	-1.14310000	-1.46040000
H	-13.67430000	0.09770000	-0.92140000
C	-11.61950000	0.77980000	-1.12720000
C	-10.25730000	0.45390000	-1.28740000
C	-9.29430000	1.47940000	-1.33280000
C	-9.70660000	2.82000000	-1.35930000
H	-8.93960000	3.57840000	-1.40240000
C	-11.07230000	3.16940000	-1.27540000
C	-12.01310000	2.12570000	-1.15540000
H	-13.06210000	2.35840000	-1.03180000
C	-11.55690000	4.63420000	-1.23860000
C	-12.25260000	4.90880000	0.11320000
H	-12.56810000	5.97230000	0.18540000
H	-11.55970000	4.69140000	0.95520000
H	-13.16080000	4.28370000	0.24160000
C	-12.55610000	4.87680000	-2.39100000
H	-12.08280000	4.63910000	-3.36840000
H	-12.88530000	5.93840000	-2.41100000
H	-13.46650000	4.25130000	-2.28320000
C	-10.40820000	5.66060000	-1.39230000
H	-9.87180000	5.51250000	-2.35450000
H	-9.68640000	5.57850000	-0.55090000
H	-10.80430000	6.69940000	-1.38630000
C	-9.89860000	-1.39460000	-2.60890000
H	-9.25450000	-0.81970000	-3.31050000
H	-10.93470000	-1.39850000	-3.01160000
C	-9.37990000	-2.82490000	-2.52320000
H	-8.28750000	-2.80580000	-2.32450000
H	-9.88740000	-3.33480000	-1.68260000
C	-9.64570000	-3.61090000	-3.80240000
H	-9.24290000	-4.64000000	-3.69350000
H	-9.15110000	-3.12620000	-4.66680000
H	-10.73680000	-3.67560000	-3.99800000
C	-7.81950000	1.15060000	-1.25790000
H	-7.19710000	2.03950000	-1.49970000
H	-7.59100000	0.38510000	-2.02280000
O	0.89910000	-1.27040000	1.38510000

O	-3.09520000	-0.53880000	1.86570000
O	-2.70760000	2.06080000	-2.24140000
O	-1.11600000	-4.03500000	-3.71860000
O	3.84470000	-4.30710000	0.25310000
O	6.40580000	-6.85620000	0.81890000
O	7.86650000	-6.79020000	3.70560000
O	5.90060000	-4.12250000	3.46270000
O	1.06130000	4.20220000	0.37400000
O	1.79920000	7.82130000	2.00320000
O	1.97700000	10.22750000	0.07160000
O	1.67120000	7.19580000	-1.52360000
O	-6.40980000	-1.33590000	-0.73420000
O	-8.94530000	-3.67780000	1.13180000
O	-11.84330000	-2.95790000	0.07860000
O	-9.86540000	-0.81050000	-1.30060000
P	1.43080000	-4.06770000	-0.99120000
P	-0.56010000	2.07200000	0.63580000
P	-4.38620000	-1.61410000	-2.54450000
Ir	0.46830000	-0.11720000	-2.72250000
Ir	-0.32520000	-2.46530000	-1.21800000
Ir	-1.20810000	0.04260000	-0.44840000
Ir	-2.16080000	-0.81310000	-2.90340000
C	0.87630000	-1.16910000	-4.27970000
O	1.13300000	-1.76560000	-5.23630000
C	2.10680000	0.11240000	-1.75320000
O	3.12180000	0.26280000	-1.21480000
C	0.24880000	1.59830000	-3.55460000
O	0.15030000	2.60540000	-4.11040000
C	-2.44370000	-0.45760000	-4.71240000
O	-2.60810000	-0.19840000	-5.83200000
C	-1.66470000	-3.62900000	0.07540000
C	-1.31580000	-3.78930000	1.55530000
H	-1.82690000	-4.60660000	-0.38500000
H	-2.61060000	-3.09300000	-0.00870000
H	-2.02520000	-4.47260000	2.04400000
H	-0.31270000	-4.19400000	1.72850000
H	-1.36280000	-2.83930000	2.09420000

Tetrairidium-trimethylphosphine complex

0 1

C	0.05520000	-1.83040000	-1.50590000
C	-2.09490000	1.24820000	0.31010000
C	2.06460000	1.29120000	0.38600000
O	0.08400000	-2.88510000	-2.03500000
O	-3.13150000	1.72640000	0.61030000
O	3.08210000	1.77870000	0.72840000

P	3.29690000	-1.71910000	-0.62940000
P	-3.27380000	-1.74480000	-0.61880000
P	-0.03300000	3.63920000	-0.69740000
Ir	0.00390000	-0.95390000	1.58470000
Ir	1.38320000	-0.34170000	-0.79740000
Ir	-1.35600000	-0.38260000	-0.81870000
Ir	-0.01510000	1.64840000	0.58730000
C	-3.06800000	-3.49550000	-1.15040000
H	-2.72980000	-3.52880000	-2.18900000
H	-2.30860000	-3.98300000	-0.53490000
H	-4.01620000	-4.03550000	-1.05560000
C	-4.04070000	-1.90210000	1.04870000
H	-3.36770000	-2.43430000	1.72350000
H	-4.23440000	-0.90930000	1.46170000
H	-4.98390000	-2.45350000	0.97210000
C	-4.70500000	-1.17140000	-1.63210000
H	-4.43350000	-1.15640000	-2.69090000
H	-5.56760000	-1.83160000	-1.49290000
H	-4.97700000	-0.15630000	-1.32930000
C	-1.11370000	4.95580000	0.00530000
H	-0.75130000	5.24030000	0.99690000
H	-1.12420000	5.83980000	-0.64090000
H	-2.13130000	4.57020000	0.11200000
C	1.59920000	4.47820000	-0.85590000
H	1.49100000	5.43370000	-1.37970000
H	2.02130000	4.65020000	0.13750000
H	2.29120000	3.83970000	-1.41070000
C	-0.61490000	3.53710000	-2.44240000
H	-0.00900000	2.82100000	-3.00120000
H	-1.65440000	3.20260000	-2.46800000
H	-0.54460000	4.52050000	-2.92010000
C	4.70840000	-1.04100000	0.33730000
H	5.01380000	-0.08000000	-0.08370000
H	4.40070000	-0.87010000	1.37160000
H	5.55320000	-1.73770000	0.31740000
C	4.06360000	-2.12140000	-2.25830000
H	4.37960000	-1.20260000	-2.75950000
H	4.93170000	-2.77690000	-2.13040000
H	3.32430000	-2.62250000	-2.88940000
C	3.05240000	-3.39400000	0.09490000
H	2.25030000	-3.90960000	-0.43840000
H	3.97670000	-3.97570000	0.01120000
H	2.77320000	-3.31000000	1.14680000
C	-1.85190000	0.22140000	-2.52150000
O	-2.13870000	0.58820000	-3.58590000
C	1.88130000	0.38670000	-2.44870000

O	2.15510000	0.87190000	-3.46900000
C	-0.04190000	2.58780000	2.19730000
O	-0.04960000	3.13900000	3.21880000
C	1.57810000	-0.72960000	2.66270000
O	2.52270000	-0.64400000	3.32700000
C	-0.15750000	-2.84150000	1.36460000
O	-0.28570000	-3.99200000	1.27600000
C	-1.41730000	-0.51480000	2.80400000
O	-2.24320000	-0.26610000	3.57460000

Π-bound Ethylene at the Apical 1on the trimethyphosphine substituted Ir cluster

0 1

C	-0.16720000	-1.82240000	-1.49440000
C	-1.83990000	1.63360000	0.22980000
C	2.21350000	0.91860000	0.50310000
O	-0.31400000	-2.87610000	-2.00820000
O	-2.79410000	2.29720000	0.42950000
O	3.28450000	1.20160000	0.92030000
P	3.03790000	-2.18680000	-0.63530000
P	-3.47300000	-1.20590000	-0.82830000
P	0.63880000	3.61570000	-0.65770000
Ir	-0.22850000	-0.93420000	1.57270000
Ir	1.34170000	-0.54800000	-0.75970000
Ir	-1.35050000	-0.16340000	-0.85140000
Ir	0.23560000	1.63290000	0.61900000
C	-0.46320000	-2.80300000	1.44040000
O	-0.67850000	-3.94460000	1.36310000
C	-1.78430000	-0.35120000	2.50650000
O	-2.75280000	-0.05040000	3.06970000
C	-3.78870000	-2.20420000	-2.34630000
H	-3.75010000	-1.55960000	-3.22880000
H	-3.00910000	-2.96480000	-2.44320000
H	-4.76990000	-2.68840000	-2.29840000
C	-3.88090000	-2.40660000	0.50780000
H	-3.14410000	-3.21210000	0.52290000
H	-3.87610000	-1.90720000	1.47820000
H	-4.87500000	-2.82990000	0.32690000
C	-4.90400000	-0.04650000	-0.78210000
H	-4.86640000	0.61540000	-1.65170000
H	-5.85040000	-0.59750000	-0.78760000
H	-4.84400000	0.57400000	0.11540000
C	-0.12790000	5.12370000	0.07670000
H	0.28290000	5.29630000	1.07520000
H	0.05990000	6.00430000	-0.54700000
H	-1.20640000	4.97040000	0.17350000
C	2.40860000	4.10200000	-0.83470000

H	2.49620000	5.06760000	-1.34400000
H	2.87260000	4.16610000	0.15290000
H	2.94350000	3.34250000	-1.41080000
C	0.02980000	3.67870000	-2.39760000
H	0.49220000	2.88370000	-2.98680000
H	-1.05330000	3.53560000	-2.41630000
H	0.26990000	4.64750000	-2.84920000
C	4.51770000	-1.80800000	0.39670000
H	4.94660000	-0.85230000	0.08590000
H	4.23360000	-1.71910000	1.44710000
H	5.26610000	-2.60060000	0.29180000
C	3.80070000	-2.57460000	-2.27160000
H	4.27130000	-1.67930000	-2.68660000
H	4.55510000	-3.36240000	-2.17320000
H	3.02200000	-2.90760000	-2.96350000
C	2.54360000	-3.86580000	-0.06160000
H	1.70400000	-4.22220000	-0.66340000
H	3.38400000	-4.56150000	-0.15910000
H	2.22430000	-3.82940000	0.98110000
C	-1.68520000	0.53050000	-2.55450000
O	-1.87220000	0.95090000	-3.62210000
C	1.97060000	0.15410000	-2.38310000
O	2.33000000	0.63570000	-3.37860000
C	0.74800000	-0.83450000	3.75190000
H	0.64880000	0.19220000	4.08590000
H	0.21540000	-1.58050000	4.33170000
C	1.76770000	-1.19670000	2.88780000
H	2.05400000	-2.23840000	2.79370000
H	2.49090000	-0.46350000	2.56040000
C	0.27910000	2.50150000	2.26100000
O	0.30480000	3.00240000	3.31110000

Π-bound Ethylene at the Basal 1 position on the trimethyphosphine substituted Ir cluster
0 1

C	-0.28901500	-1.77551700	-1.53232700
C	-1.81614400	1.63174700	0.30867400
C	2.25253600	0.82457200	0.45370300
O	-0.45952000	-2.80483000	-2.08439700
O	-2.74630800	2.30832700	0.57828400
O	3.34171800	1.08681500	0.82762000
P	2.92402500	-2.27156000	-0.68398700
P	-3.54711000	-1.05219000	-0.67536900
P	0.73505900	3.52145100	-0.62305500
Ir	-0.20537000	-1.02037700	1.56597900
Ir	1.28985600	-0.57033000	-0.79031200
Ir	-1.39854500	-0.09806000	-0.82026100

Ir	0.28810600	1.61594100	0.66364700
C	1.35478100	-1.08249600	2.67171700
O	2.28091100	-1.14729300	3.36816000
C	-0.70434500	-2.84783200	1.28415000
O	-1.04903500	-3.95179600	1.17753400
C	-1.54605600	-0.32828700	2.73458700
O	-2.33513100	0.07625100	3.48344700
C	-3.72547400	-2.69153300	-1.49514400
H	-3.43033100	-2.61245100	-2.54438700
H	-3.06499800	-3.41761500	-1.01519000
H	-4.76171200	-3.04004200	-1.43011100
C	-4.28225500	-1.34438200	0.98713400
H	-3.68691000	-2.07416900	1.53839400
H	-4.30364600	-0.41128100	1.55436800
H	-5.30410600	-1.72244300	0.87384400
C	-4.85813600	-0.03444800	-1.48040300
H	-4.63649000	0.09281800	-2.54328300
H	-5.83907500	-0.50952800	-1.37382400
H	-4.88201500	0.95268400	-1.00981900
C	0.24465800	5.15900400	0.08393200
H	0.73943800	5.33137600	1.04350300
H	0.52684600	5.96218600	-0.60441500
H	-0.83735100	5.18852300	0.23890200
C	2.51394800	3.80482500	-1.02609200
H	2.63884800	4.74980500	-1.56513000
H	3.10848300	3.82609200	-0.10938100
H	2.88474700	2.98785400	-1.64962200
C	-0.05333300	3.59863300	-2.28723900
H	0.25624200	2.73952000	-2.88496700
H	-1.14082000	3.57557200	-2.18521700
H	0.23949800	4.51998300	-2.80211500
C	4.36269900	-1.97895800	0.42679000
H	4.85222100	-1.04075600	0.15549600
H	4.02643600	-1.89281300	1.46248500
H	5.07627900	-2.80550400	0.34316300
C	3.73865700	-2.63182100	-2.30073600
H	4.25470000	-1.74008200	-2.66631300
H	4.46364200	-3.44570700	-2.19489200
H	2.98170200	-2.92002400	-3.03540800
C	2.33706500	-3.94189700	-0.17919600
H	1.48863800	-4.23651900	-0.80140400
H	3.14409300	-4.67387400	-0.29154100
H	2.01233500	-3.91960100	0.86248900
C	-1.76408200	0.60425000	-2.52020900
O	-1.97813000	1.01261900	-3.58693600
C	1.90217500	0.10817900	-2.42759200

O	2.25225600	0.56443700	-3.43801100
C	1.13550500	2.59309800	2.44963400
H	1.56958200	1.83734900	3.09585000
H	1.81791500	3.39985900	2.19490000
C	-0.26154100	2.80118000	2.44105500
H	-0.67731000	3.76425700	2.16710200
H	-0.90213800	2.21045400	3.08536800

Ethyl bound at the Apical 3 position on the trimethylphosphine substituted Ir cluster
0 2

C	0.78050000	1.28550000	-1.85920000
C	1.04230000	-2.02370000	0.59610000
C	-2.49800000	0.13070000	0.46740000
O	1.29370000	2.10240000	-2.53950000
O	1.71210000	-2.86330000	1.08960000
O	-3.60480000	0.32780000	0.82320000
P	-1.74250000	3.21330000	-0.74370000
P	3.53280000	-0.57080000	-1.11860000
P	-2.04750000	-3.09290000	-0.17660000
Ir	0.76100000	0.86950000	1.40350000
Ir	-1.09280000	0.94170000	-0.91570000
Ir	1.17860000	-0.58520000	-0.95140000
Ir	-0.92450000	-1.23200000	0.80930000
C	4.28560000	0.91860000	-1.89790000
H	3.85690000	1.06980000	-2.89140000
H	4.06700000	1.80420000	-1.29730000
H	5.37050000	0.79320000	-1.98010000
C	4.50120000	-0.76110000	0.43660000
H	4.35870000	0.11510000	1.07200000
H	4.15510000	-1.64750000	0.97430000
H	5.56650000	-0.86810000	0.20600000
C	4.21640000	-1.94420000	-2.14620000
H	3.81890000	-1.88380000	-3.16280000
H	5.30950000	-1.89060000	-2.18620000
H	3.92030000	-2.90450000	-1.71480000
C	-1.02730000	-4.60990000	-0.41340000
H	-0.57000000	-4.89780000	0.53670000
H	-1.64450000	-5.43420000	-0.78640000
H	-0.22750000	-4.40960000	-1.13070000
C	-3.47680000	-3.71130000	0.81030000
H	-3.97020000	-4.54660000	0.30200000
H	-3.13040000	-4.04280000	1.79290000
H	-4.19590000	-2.90050000	0.95660000
C	-2.79660000	-2.83790000	-1.84190000
H	-3.54030000	-2.03850000	-1.79230000
H	-2.02340000	-2.54620000	-2.55570000

H	-3.28100000	-3.75740000	-2.18820000
C	-3.03360000	3.60680000	0.50780000
H	-3.92780000	3.00870000	0.31610000
H	-2.67040000	3.35900000	1.50790000
H	-3.28710000	4.67150000	0.46710000
C	-2.44320000	3.92890000	-2.29310000
H	-3.34680000	3.38560000	-2.58220000
H	-2.69120000	4.98610000	-2.15200000
H	-1.71070000	3.83630000	-3.09990000
C	-0.38970000	4.39880000	-0.35150000
H	0.41670000	4.28670000	-1.08060000
H	-0.76780000	5.42660000	-0.38080000
H	0.00910000	4.18630000	0.64220000
C	0.95290000	-1.71690000	-2.43740000
O	0.77500000	-2.44010000	-3.33010000
C	-2.09320000	0.67400000	-2.47230000
O	-2.70260000	0.50920000	-3.44840000
C	-1.31230000	-1.74860000	2.55850000
O	-1.53430000	-2.04300000	3.65990000
C	-0.44620000	1.60760000	2.65690000
O	-1.18650000	2.14750000	3.37150000
C	2.12580000	2.11400000	1.04370000
O	2.93520000	2.92540000	0.83240000
C	1.90330000	0.04140000	3.07930000
C	2.48440000	1.00660000	4.09920000
H	2.68480000	-0.52600000	2.57100000
H	1.20740000	-0.65660000	3.54740000
H	3.03050000	0.45270000	4.87780000
H	3.18800000	1.71470000	3.64770000
H	1.70560000	1.58910000	4.60280000

Ethyl bound at the Basal 2 position on the trimethylphosphine substituted Ir cluster
0 2

C	-0.28664800	-1.78272400	-1.58792800
C	-1.55585800	1.84186900	0.21943300
C	2.52507300	0.43460500	0.21359900
O	-0.60086300	-2.73098900	-2.22146500
O	-2.42082600	2.60654500	0.47760400
O	3.60921900	0.79280300	0.49950600
P	2.47107300	-2.77615600	-0.23066400
P	-3.56679800	-0.61553900	-1.09280700
P	1.18774100	3.40551800	-0.69840900
Ir	-0.64710400	-0.74132800	1.71071200
Ir	1.25596300	-0.82726400	-0.64213600
Ir	-1.30081600	0.07129900	-0.94686300
Ir	0.47053500	1.55451600	0.56154000

C	-3.88462500	-2.33523400	-1.67148600
H	-3.39421400	-2.48775000	-2.63606900
H	-3.46088600	-3.05053600	-0.96339700
H	-4.96062100	-2.51373500	-1.77147600
C	-4.57466100	-0.48238400	0.44482700
H	-4.20189500	-1.17482800	1.20146000
H	-4.50119100	0.53553700	0.83645900
H	-5.62390500	-0.71377100	0.23177200
C	-4.56976300	0.39192900	-2.27089400
H	-4.16022500	0.30623900	-3.28088800
H	-5.61196700	0.05560800	-2.27865300
H	-4.53325200	1.44273700	-1.97013200
C	-0.04300600	4.76612000	-0.84822300
H	-0.35544300	5.08763600	0.14856000
H	0.38680100	5.61540000	-1.38972900
H	-0.92801000	4.40819000	-1.37983700
C	2.66815700	4.25002000	0.00089500
H	2.99330100	5.06820600	-0.65039700
H	2.42966500	4.65108800	0.98956600
H	3.47974400	3.52609700	0.11284700
C	1.68549300	3.10218200	-2.44565500
H	2.50593100	2.38207300	-2.47330800
H	0.84665900	2.69344200	-3.01213400
H	2.01265500	4.03898600	-2.90974200
C	4.08070000	-2.57030100	0.64446400
H	4.73993100	-1.90991800	0.07628000
H	3.90770400	-2.11275000	1.62210400
H	4.56675900	-3.54194100	0.78105600
C	2.90838300	-3.83163600	-1.68114500
H	3.58876600	-3.30744200	-2.35486700
H	3.38753000	-4.75458300	-1.33885900
H	1.99517200	-4.08040300	-2.22903600
C	1.60269500	-4.00598200	0.83376600
H	0.66621100	-4.30844500	0.35897300
H	2.23451900	-4.88953800	0.97558300
H	1.37356400	-3.56813100	1.80681700
C	-1.36008400	0.85303100	-2.62700600
O	-1.36384300	1.37424600	-3.66916000
C	0.89684800	-0.77370000	2.85163500
O	1.82342000	-0.86813200	3.54006300
C	-1.50882200	-2.39833400	1.32654600
O	-2.01504400	-3.42854300	1.14603800
C	-1.90213500	-0.06711000	2.98408800
O	-2.65460100	0.31541600	3.77334600
C	0.86620000	2.43486900	2.15907600
O	1.08580500	2.95621900	3.17490800

C	2.20813300	-0.72651700	-2.58519400
C	3.69162100	-0.37992700	-2.66913600
H	1.61587600	0.05217100	-3.07773800
H	2.00900100	-1.66056700	-3.11701700
H	4.00817300	-0.31259700	-3.72078900
H	3.92983100	0.57625600	-2.19373000
H	4.33061300	-1.13143800	-2.19264900

$Ir_4(CO)_9(PPh_2CH_2OCH_3)_3$

Ir	-0.49314338	-1.17853470	-0.64942544
P	-2.08078151	-2.83201481	-0.91059261
C	-1.75314022	0.40594906	-1.06686505
C	-3.03031916	-2.48196231	-2.47864085
C	-3.34926483	-2.94023866	0.37718400
C	-1.50032428	-4.52144415	-1.20020509
C	0.15646558	-1.52203297	-2.33618163
C	0.78429779	-2.23597465	0.60366341
Ir	-0.10147849	1.46143653	-0.35764561
O	-2.85423607	0.58079170	-1.49582142
O	-3.91987347	-3.46014622	-2.91423540
H	-2.24588945	-2.38008139	-3.25466510
H	-3.51140669	-1.48448729	-2.34927294
C	-4.25016824	-1.87232746	0.49294596
C	-3.40151913	-3.99738028	1.29095725
C	-0.14636261	-4.78531335	-1.42995143
C	-2.43688718	-5.55961537	-1.31709768
O	0.55880892	-1.67641427	-3.42654155
O	0.96418056	-3.33680767	1.01112673
P	-1.05122813	3.49369573	0.14190447
C	1.55272492	1.72985063	0.86577193
C	0.52679939	2.09744324	-1.97041502
C	-5.18741731	-3.42927517	-2.29936437
C	-5.21446797	-1.88103940	1.49537188
H	-4.18779727	-1.01320818	-0.19489942
C	-4.37236889	-4.00161359	2.29220268
H	-2.66974741	-4.81515140	1.22889056
C	0.26767413	-6.07408791	-1.75973057
H	0.59889043	-3.98257536	-1.34076269
C	-2.01744055	-6.84597051	-1.64499793
H	-3.50485473	-5.35986284	-1.15074255
C	-0.92029933	3.90099980	1.92616788
C	-2.80069967	3.68672767	-0.26342700
C	-0.25355509	4.93379230	-0.63063425

Ir	1.58281373	-0.33377543	0.86709273
O	2.17824237	2.62283293	1.35922442
O	0.90173252	2.49651198	-3.00530166
H	-5.16826292	-3.83662611	-1.26613027
H	-5.85963228	-4.04576703	-2.92021082
H	-5.58457275	-2.39237527	-2.24771353
C	-5.28312541	-2.95032416	2.39239262
H	-5.90489328	-1.03193173	1.58605249
H	-4.40403367	-4.83041142	3.01155932
C	-0.66358472	-7.10595012	-1.86515907
H	1.33761786	-6.26143273	-1.92787175
H	-2.75660097	-7.65306372	-1.73453985
O	-1.28802751	5.22963764	2.15936122
H	-1.55370052	3.17837932	2.49361869
H	0.14124365	3.70683441	2.20941096
C	-3.73301078	4.13389566	0.67877094
C	-3.21559228	3.38118229	-1.56449438
C	-1.00588901	5.97980443	-1.17124891
C	1.14453870	5.00087771	-0.64094166
P	3.36434007	-0.63163118	-0.54433059
C	2.58025374	-0.64022030	2.38429677
H	-6.04187491	-2.95403337	3.18619476
H	-0.33483081	-8.12213595	-2.12142650
C	-0.97118804	5.61414727	3.47693729
C	-5.07247856	4.26951356	0.31795320
H	-3.40147595	4.41277880	1.68871919
C	-4.55105508	3.53556319	-1.92489659
H	-2.48506507	3.01378466	-2.29968274
C	-0.36190875	7.08177460	-1.73267220
H	-2.10400235	5.92989805	-1.15303292
C	1.78183422	6.10954157	-1.19242261
H	1.73738220	4.18621061	-0.19701766
C	3.22457507	0.39334814	-2.05716853
C	3.54833600	-2.33128030	-1.13562277
C	4.99530472	-0.17738900	0.09922158
O	3.18061711	-0.84611850	3.36437723
H	-1.27611811	6.66705414	3.59564455
H	0.11968658	5.52408579	3.66828600
H	-1.50875062	4.98933069	4.22359050
C	-5.48244340	3.97373170	-0.98231307
H	-5.80259449	4.61741409	1.06059958
H	-4.86907446	3.29353784	-2.94746461
C	1.03098631	7.14874225	-1.74471386
H	-0.95700784	7.89808637	-2.16326524
H	2.87886453	6.16000099	-1.19359563
O	4.34266033	0.23655645	-2.87756037

H	2.27562397	0.12369940	-2.57777406
H	3.11064164	1.44549817	-1.70125317
C	3.73784855	-3.33567245	-0.17739683
C	3.43115259	-2.67123170	-2.48753889
C	6.14848488	-0.79580220	-0.39556281
C	5.09683312	0.84727599	1.04646167
H	-6.53819251	4.08507413	-1.26379797
H	1.53586449	8.01772028	-2.18754747
C	4.27808594	1.11611816	-3.97792239
C	3.82763910	-4.66742086	-0.57090793
H	3.79848104	-3.07294292	0.88925575
C	3.50636635	-4.00892944	-2.87532416
H	3.30203532	-1.88662129	-3.24536921
C	7.40024115	-0.39632366	0.06710735
H	6.05932974	-1.59606335	-1.14418169
C	6.35295097	1.24617493	1.49955765
H	4.18972111	1.33980497	1.43026522
H	5.17723022	0.94344078	-4.59204551
H	4.25932876	2.17536923	-3.64209504
H	3.36878391	0.93114963	-4.59020096
C	3.71012081	-5.00599898	-1.92089507
H	3.97154737	-5.44863733	0.18668438
H	3.40850381	-4.27136121	-3.93695316
C	7.50342951	0.62345461	1.01467827
H	8.30505320	-0.88664143	-0.31584829
H	6.43036315	2.04652090	2.24713793
H	3.78680927	-6.05716616	-2.23251896
H	8.49125744	0.93304610	1.38143047
C	-2.72196405	0.62086969	1.64950967
Ir	-0.95718637	-0.00146849	1.81724963
O	-3.80574266	1.05214734	1.59971821
C	-1.16619449	-1.69965540	2.62086274
C	-0.16788785	1.05443761	3.16197142
O	-1.32731179	-2.72987936	3.13700353
O	0.31574472	1.67901969	4.02100719

$Ir4(CO)_8(C_2H_4)(PPh_2CH_2OCH_3)_3$
Apical.1.C_2H_4

Ir	-1.12581400	-0.56310700	0.57080100
P	-2.66331600	-2.27271200	0.78522900
C	0.49875900	-1.57688500	1.36394500
C	-2.42663800	-3.07149800	2.45403700
C	-2.55473500	-3.63327000	-0.40374600
C	-4.41414400	-1.81298700	0.85254400
C	-1.72457400	0.20205700	2.13827500
C	-2.16422400	0.52844000	-0.87272200

Ir	1.48389000	0.06521300	0.53281300
O	0.70606800	-2.57049600	1.99130300
O	-3.39190100	-3.98996700	2.85913000
H	-2.46248900	-2.22286800	3.16581900
H	-1.39169600	-3.48526000	2.48103900
C	-1.46826300	-4.51271400	-0.30967000
C	-3.47033500	-3.76943500	-1.45212300
C	-4.79908100	-0.47393400	0.96846800
C	-5.39066100	-2.81909500	0.90917400
O	-2.04072700	0.69552400	3.15421800
O	-3.23196900	0.57201700	-1.39038300
P	3.63763200	-0.69681200	0.34873000
C	1.71823200	1.61755100	-0.80877000
C	1.87215700	0.91282900	2.13308000
C	-3.20305200	-5.30500800	2.39052500
C	-1.31862500	-5.53805600	-1.23794500
H	-0.71750900	-4.38726600	0.48581300
C	-3.31756400	-4.79999700	-2.37835100
H	-4.30041400	-3.05623200	-1.55264700
C	-6.14342100	-0.14227900	1.12396000
H	-4.04506700	0.32362000	0.92429200
C	-6.73299000	-2.48308000	1.06294300
H	-5.09952900	-3.87604300	0.82921100
C	4.29467900	-0.53216400	-1.35284500
C	3.94510200	-2.41094000	0.82480100
C	4.86962000	0.26862000	1.27562500
Ir	-0.32534200	1.47464000	-1.00209000
O	2.60463200	2.27759600	-1.27926800
O	2.13551100	1.43136100	3.14986800
H	-3.47094500	-5.41810300	1.31881700
H	-3.85363600	-5.95692300	2.99784600
H	-2.14656000	-5.62788700	2.51352700
C	-2.24808100	-5.68893400	-2.27032000
H	-0.45679100	-6.21374100	-1.16057200
H	-4.03632900	-4.89757600	-3.20227400
C	-7.11242300	-1.14345600	1.16829400
H	-6.42321300	0.91767800	1.20239600
H	-7.49067500	-3.27652400	1.10534400
O	5.65384100	-0.85755900	-1.40705000
H	3.67693500	-1.17041900	-2.02771800
H	4.11634100	0.53338900	-1.63357800
C	4.55739800	-3.32292300	-0.04202200
C	3.53965800	-2.82492900	2.09909600
C	5.86500300	-0.33984300	2.04339700
C	4.82484700	1.66415300	1.16784700
P	-0.91264500	3.34326400	0.20202300

C	-0.52397800	2.28464100	-2.64072300
H	-2.12811000	-6.49683500	-3.00411900
H	-8.17237500	-0.88125200	1.28573000
C	6.22742900	-0.44728600	-2.62524300
C	4.75705800	-4.64062100	0.36525800
H	4.91717200	-2.98724300	-1.02431800
C	3.75680000	-4.13816100	2.50687700
H	3.04261900	-2.11536700	2.77508500
C	6.80431300	0.44507500	2.71228800
H	5.90449600	-1.43613600	2.11567200
C	5.77358300	2.44212300	1.82630000
H	4.04564100	2.14315500	0.55336100
C	-0.05791400	3.44543100	1.82144300
C	-2.67588200	3.43661700	0.60205400
C	-0.52101200	4.94404300	-0.55307200
O	-0.63985100	2.74071000	-3.71269900
H	7.29346900	-0.72689300	-2.59865100
H	6.14144500	0.65297600	-2.75676500
H	5.74059600	-0.94398800	-3.49340200
C	4.35974800	-5.04941000	1.63868600
H	5.23623600	-5.35409500	-0.31786500
H	3.43527700	-4.45507200	3.50749000
C	6.76119900	1.83480800	2.60466500
H	7.58056300	-0.03651000	3.32143300
H	5.73746300	3.53573500	1.73495600
O	-0.37899800	4.63316700	2.48192900
H	-0.32231100	2.54589100	2.42704900
H	1.03229700	3.37492900	1.59323300
C	-3.58706900	3.44398100	-0.46242400
C	-3.14715600	3.41085600	1.91920500
C	-1.26853000	6.08177500	-0.22928100
C	0.57113200	5.04449600	-1.42199400
H	4.52205600	-6.08746400	1.95784600
H	7.50242300	2.45031000	3.13135200
C	0.36292900	4.75802400	3.67412700
C	-4.95598500	3.44590100	-0.21113600
H	-3.21953900	3.43050800	-1.49899600
C	-4.51995800	3.39680500	2.16619300
H	-2.44042800	3.42288100	2.75989200
C	-0.92898500	7.31427600	-0.78263800
H	-2.12363600	5.99496600	0.45605500
C	0.90984800	6.28252500	-1.96579100
H	1.16328700	4.15035800	-1.67283100
H	0.06809400	5.70844700	4.14827200
H	1.45447100	4.77280600	3.46610200
H	0.15490100	3.91604800	4.36971200

C	-5.42480200	3.41993300	1.10438900
H	-5.66178000	3.44686500	-1.05166900
H	-4.88345400	3.37100300	3.20172700
C	0.15925100	7.41583400	-1.65109300
H	-1.52077600	8.20511300	-0.53434900
H	1.76461800	6.35811400	-2.65049200
H	-6.50549100	3.42486000	1.30316000
H	0.42177100	8.38764000	-2.08982700
C	0.99888300	-2.72377900	-1.10131600
Ir	0.30936400	-1.09228900	-1.71677700
O	1.45175300	-3.75640600	-0.78938800
C	-1.24842900	-1.41619100	-2.70714900
O	-2.22154000	-1.69967400	-3.28857300
C	1.50369100	-0.12045200	-3.32579700
H	0.84605600	0.46493600	-3.97983200
H	2.36672500	0.43056500	-2.93152200
C	1.55929200	-1.51804000	-3.49288600
H	0.94800300	-2.00910300	-4.26049400
H	2.46609600	-2.07606500	-3.21888300

$Ir4(CO)_8(C_2H_4)(PPh_2CH_2OCH_3)_3$
Apical.2.C_2H_4

Ir	1.17659900	-0.53802300	-0.54829400
P	2.79596400	-2.16345400	-0.75785100
C	-0.40043200	-1.68600300	-1.23495600
C	2.63918300	-2.91929700	-2.45656800
C	2.74416100	-3.55243400	0.40293700
C	4.52449500	-1.62055700	-0.76649000
C	1.72772700	0.21478600	-2.13545400
C	2.13646600	0.63381200	0.87590700
Ir	-1.46727200	-0.02653500	-0.56911000
O	-0.55378700	-2.74382100	-1.77246100
O	3.68212100	-3.73341900	-2.89085200
H	2.61044100	-2.04039300	-3.13053100
H	1.64030000	-3.41222600	-2.51367100
C	1.83943600	-4.60211100	0.19116800
C	3.54208000	-3.54996800	1.55385600
C	4.84869900	-0.26777100	-0.90809700
C	5.54794800	-2.57905000	-0.75426500
O	2.00954300	0.68737500	-3.17245500
O	3.19574500	0.75922400	1.39678300
P	-3.58673200	-0.87587400	-0.37365800
C	-1.81082500	1.57832100	0.69271700
C	-1.85088400	0.73378500	-2.21415300
C	3.59774200	-5.08421400	-2.50552300
C	1.75449500	-5.64971400	1.10652000

H	1.19887500	-4.60692500	-0.70417800
C	3.45116300	-4.59780600	2.46744100
H	4.23408700	-2.71657600	1.73961300
C	6.18133900	0.12309800	-1.02191400
H	4.05773300	0.49508500	-0.91658200
C	6.87807300	-2.18405400	-0.86699700
H	5.30190300	-3.64536500	-0.64666800
C	-4.19173400	-0.86811400	1.35813800
C	-3.82602500	-2.58241700	-0.93123700
C	-4.89897500	0.04120100	-1.23692900
Ir	0.23538800	1.47642000	0.98882000
O	-2.72356400	2.24700400	1.08354200
O	-2.10061900	1.18587800	-3.26606300
H	3.82109500	-5.23524400	-1.42839300
H	4.33945200	-5.63450900	-3.10872800
H	2.58625200	-5.49900500	-2.70911400
C	2.56240400	-5.65088100	2.24506200
H	1.04425100	-6.46809100	0.92964600
H	4.07739300	-4.58361500	3.36884200
C	7.19735600	-0.83114500	-0.99922700
H	6.41420700	1.19288000	-1.11845500
H	7.67371000	-2.94049600	-0.85510100
O	-5.55221200	-1.18647900	1.42298000
H	-3.55977900	-1.58072800	1.94346600
H	-3.98796700	0.15366500	1.75298600
C	-4.46362600	-3.54492400	-0.13764300
C	-3.35567400	-2.93295400	-2.20263000
C	-5.94180200	-0.62575400	-1.88678500
C	-4.87965200	1.44019300	-1.20350700
P	0.76265400	3.34312900	-0.24367600
C	0.38748200	2.34546900	2.60900500
H	2.49488400	-6.47585100	2.96628600
H	8.24753000	-0.52119000	-1.08353100
C	-6.06232800	-0.94772600	2.71460400
C	-4.62002100	-4.84614200	-0.61402500
H	-4.87550800	-3.25983100	0.84085100
C	-3.53166300	-4.22840300	-2.68101400
H	-2.84092200	-2.18457600	-2.82154400
C	-6.95401000	0.10349000	-2.50899700
H	-5.96016300	-1.72463500	-1.90711000
C	-5.89989200	2.16327700	-1.81727800
H	-4.06979700	1.96564200	-0.67540600
C	-0.03999700	3.36097400	-1.89233900
C	2.53145100	3.51525100	-0.58331300
C	0.26680600	4.94170000	0.45129100
O	0.49424700	2.86020400	3.65251500

H	-7.13508100	-1.20082200	2.69763600
H	-5.93966900	0.11831100	3.00174400
H	-5.54850300	-1.57430700	3.47656500
C	-4.15769400	-5.18899100	-1.88525000
H	-5.11895400	-5.59751500	0.01207900
H	-3.15911800	-4.49296100	-3.67908900
C	-6.93559000	1.49777100	-2.47509400
H	-7.76718800	-0.42505800	-3.02371600
H	-5.88289000	3.26056800	-1.78289300
O	0.25187200	4.54373900	-2.57495400
H	0.28604000	2.45898300	-2.46147100
H	-1.13401000	3.24682800	-1.70158400
C	3.39451500	3.62702200	0.51436200
C	3.05655700	3.45353800	-1.87859300
C	0.93896300	6.11019500	0.07431300
C	-0.83282100	5.00986800	1.31334800
H	-4.28726500	-6.21338500	-2.25887100
H	-7.73421600	2.07021800	-2.96520700
C	-0.45410000	4.60264300	-3.79393800
C	4.76998200	3.69812800	0.31648800
H	2.98452700	3.63890500	1.53514100
C	4.43710300	3.50994600	-2.07121800
H	2.38565700	3.38274000	-2.74542700
C	0.51691700	7.34163200	0.56979600
H	1.79801300	6.04833700	-0.60876400
C	-1.25309100	6.24661300	1.80040900
H	-1.37066300	4.09297400	1.59941800
H	-0.18295500	5.55052700	-4.28690900
H	-1.55171900	4.57772200	-3.62186800
H	-0.18808400	3.75032700	-4.45625200
C	5.29363800	3.63806600	-0.97710400
H	5.43948100	3.78078600	1.18217100
H	4.84426100	3.45817500	-3.08944900
C	-0.57774800	7.41088500	1.43367900
H	1.04853200	8.25735000	0.27951900
H	-2.11345100	6.29653300	2.48037300
H	6.37952600	3.69979100	-1.13354300
H	-0.90512300	8.38247300	1.82701600
Ir	-0.32940900	-1.06582900	1.74336800
C	1.28801200	-1.35518600	2.64550500
C	-1.54977400	-0.21731600	2.88298200
O	2.25904000	-1.50217200	3.28009000
O	-2.25111000	0.30560700	3.66178600
C	-0.96658700	-3.09605700	1.17337600
H	-1.86885700	-3.09557000	0.54725500
H	-0.11568000	-3.65461700	0.76405700

C	-1.07706400	-2.95613300	2.57220800
H	-0.32350500	-3.41003000	3.22986100
H	-2.06721300	-2.83120000	3.03415400

$Ir4(CO)_8(C_2H_4)(PPh_2CH_2OCH_3)_3$
$Axial.C_2H_4$

Ir	1.14979100	-0.55062200	-0.73714900
P	2.90102900	-2.04813500	-0.71141200
C	-0.37733600	-1.73816300	-1.39067100
C	2.54690200	-3.47835300	-1.85541500
C	3.33809300	-2.84095200	0.86535600
C	4.50737900	-1.38843200	-1.26905800
C	2.16251400	0.60890700	0.58387500
Ir	-1.50446700	-0.14387100	-0.56981300
O	-0.55237000	-2.76748900	-1.96853500
O	3.57296200	-4.38159300	-2.13617000
H	2.25443700	-3.00991300	-2.81390500
H	1.63309700	-3.97990000	-1.46023300
C	2.52025700	-3.85745800	1.37687800
C	4.45421700	-2.42225300	1.59665100
C	4.67343900	-0.01659800	-1.48764400
C	5.59542600	-2.24998400	-1.47027900
O	3.21960300	0.71754100	1.12717700
P	-3.56195300	-1.13189200	-0.29951300
C	-1.82607100	1.40045200	0.76647700
C	-2.04964900	0.66660800	-2.13405900
C	3.74647800	-5.41542700	-1.19367600
C	2.83259700	-4.46794000	2.58662400
H	1.62477200	-4.18278900	0.82768200
C	4.75993700	-3.03154400	2.81397500
H	5.08307200	-1.60590100	1.21524700
C	5.90211600	0.48946700	-1.90494600
H	3.83171500	0.66793800	-1.30978600
C	6.82243800	-1.74171600	-1.89318700
H	5.47745700	-3.32867700	-1.30488600
C	-4.13689500	-1.12673000	1.44252800
C	-3.72065800	-2.85429600	-0.82504200
C	-4.93483400	-0.27205300	-1.12789000
Ir	0.22368900	1.43291000	0.88810700
O	-2.74877100	2.00224600	1.24361500
O	-2.38631500	1.18933900	-3.12909100
H	4.26360700	-5.07081300	-0.27363000
H	4.35514400	-6.19437900	-1.68376600
H	2.76998200	-5.85304400	-0.89413600
C	3.95681900	-4.05775200	3.30807100
H	2.18547700	-5.26599700	2.97393000

H	5.63090800	-2.68816800	3.38704700
C	6.97977400	-0.37190500	-2.11075300
H	6.00627400	1.57193100	-2.06714300
H	7.66632500	-2.42564000	-2.05319200
O	-5.48636900	-1.48567700	1.51712200
H	-3.48587800	-1.81851200	2.02805000
H	-3.95951200	-0.09561100	1.82739900
C	-4.21382300	-3.84412800	0.03274000
C	-3.32273100	-3.19679400	-2.12279500
C	-5.86419400	-0.95540800	-1.91534000
C	-5.05985900	1.11059400	-0.94144500
P	0.46043400	3.45967500	-0.16089700
C	0.49991700	2.17822600	2.54743900
H	4.19792500	-4.53240000	4.26815100
H	7.94954700	0.02422500	-2.44025800
C	-5.99154300	-1.27330700	2.81447800
C	-4.30012600	-5.16448800	-0.40511300
H	-4.57021300	-3.57433200	1.03625600
C	-3.42839200	-4.51371400	-2.56187500
H	-2.91829200	-2.42662500	-2.79439400
C	-6.90569700	-0.25798500	-2.52747000
H	-5.77298700	-2.04281900	-2.04824400
C	-6.11034500	1.79861200	-1.54352000
H	-4.33822600	1.65071800	-0.30728200
C	-0.74005600	3.65738500	-1.53832100
C	2.08786800	3.79925200	-0.88465700
C	0.08925300	4.91674900	0.85395200
O	0.67107500	2.59195700	3.62707000
H	-7.05469500	-1.56470800	2.80597900
H	-5.90576600	-0.20477200	3.10728600
H	-5.44853900	-1.88499300	3.56813000
C	-3.90975300	-5.50116300	-1.70148200
H	-4.68426800	-5.93756900	0.27318600
H	-3.11077500	-4.77255800	-3.58023400
C	-7.03104000	1.11844200	-2.34345600
H	-7.62903800	-0.79922200	-3.15151500
H	-6.20945600	2.88114600	-1.38787500
O	-0.72062500	4.95304500	-2.06347100
H	-0.52050800	2.89052900	-2.31722800
H	-1.73749300	3.40357100	-1.10582000
C	3.21777600	3.53090200	-0.10104700
C	2.24529200	4.25133700	-2.20126600
C	0.83281600	6.09403300	0.73443500
C	-0.99798100	4.85844000	1.73433500
H	-3.98006100	-6.54219700	-2.04350900
H	-7.85261800	1.66544200	-2.82457600

C	-1.75438000	5.12170500	-3.00711500
C	4.49362000	3.69766400	-0.63497200
H	3.09960600	3.15952400	0.92642900
C	3.52519500	4.40762000	-2.73327800
H	1.35723000	4.50103100	-2.79962700
C	0.49465900	7.20922900	1.49966900
H	1.68469900	6.13484800	0.04059300
C	-1.33618800	5.97996100	2.48813500
H	-1.58550700	3.93129400	1.83150200
H	-1.68785800	6.15327100	-3.38981500
H	-2.74989600	4.96796600	-2.53745300
H	-1.65486300	4.40453800	-3.85073900
C	4.64932300	4.12737600	-1.95486200
H	5.37182000	3.47273500	-0.01533800
H	3.64450700	4.75394200	-3.76828700
C	-0.58985000	7.15416300	2.37540700
H	1.08533200	8.13041000	1.41057200
H	-2.18762200	5.93070000	3.17937300
H	5.65531300	4.25377000	-2.37805500
H	-0.85309500	8.03259800	2.97931400
C	-0.62964500	-2.93792600	1.18065700
Ir	-0.17200700	-1.15796000	1.60445900
O	-0.92719300	-4.04731600	0.96400900
C	1.36197500	-1.22565900	2.71912500
C	-1.39413100	-0.58849600	2.91575000
O	2.25080500	-1.24472800	3.46818500
O	-2.11295100	-0.23408100	3.76437600
C	1.76294800	-0.50160400	-2.82687800
H	2.82968800	-0.69249400	-3.01611300
H	1.07523300	-1.10288500	-3.44005000
C	1.36101800	0.78907200	-2.41075200
H	0.38025400	1.16332000	-2.73355700
H	2.11357500	1.57178800	-2.23372800

$Ir4(CO)_8(C_2H_4)(PPh_2CH_2OCH_3)_3$
Equatorial.C_2H_4

Ir	-1.22534800	-0.41175700	0.51447900
P	-2.85920000	-2.00627500	0.78202500
C	0.32771000	-1.49215400	1.34417600
C	-2.70107000	-2.73026100	2.49292300
C	-2.80072100	-3.43630500	-0.32842700
C	-4.58033000	-1.44288400	0.76759500
C	-1.84916400	0.42423800	2.03259000
C	-2.09295800	0.65879600	-1.12567700
Ir	1.47156700	0.01623700	0.47756600
O	0.46441500	-2.48622000	1.99500100

O	-3.70676000	-3.59295200	2.92385200
H	-2.71816200	-1.84722500	3.16200800
H	-1.68218300	-3.17914700	2.55906900
C	-1.73787500	-4.33873500	-0.18947600
C	-3.74043900	-3.61980300	-1.34714000
C	-4.88752100	-0.07965400	0.71431600
C	-5.61380100	-2.37969300	0.92214100
O	-2.20091900	0.91846300	3.03780000
O	-3.10726200	0.65467000	-1.75227700
P	3.54943200	-0.93519500	0.36570500
C	1.79936000	1.48585100	-1.06669200
C	1.99537900	0.84088500	2.03934700
C	-3.57103600	-4.92982800	2.50028300
C	-1.63263800	-5.42835300	-1.04772500
H	-0.97593400	-4.18173000	0.59048600
C	-3.63266900	-4.71576200	-2.20297100
H	-4.55516500	-2.89424500	-1.48055500
C	-6.21239600	0.34168600	0.80963900
H	-4.08518400	0.66154700	0.58570100
C	-6.93591400	-1.95336200	1.01415800
H	-5.38289600	-3.45294000	0.97071600
C	4.13250800	-1.14480800	-1.36007500
C	3.73892000	-2.56038500	1.13482100
C	4.89301200	0.05930600	1.08111100
Ir	-0.20821200	1.41912000	-1.11593700
O	2.74459400	1.97447300	-1.62188900
O	2.34794100	1.29708600	3.06159200
H	-3.84872100	-5.06776700	1.43373600
H	-4.24308400	-5.53531800	3.13186800
H	-2.52702500	-5.28884200	2.62843800
C	-2.58458100	-5.62310600	-2.05279100
H	-0.78824500	-6.12155800	-0.93787900
H	-4.36934800	-4.85041600	-3.00558900
C	-7.23761000	-0.59119500	0.95847700
H	-6.43313800	1.41736100	0.76586500
H	-7.73875000	-2.69225300	1.13626200
O	5.48895200	-1.48384800	-1.39471000
H	3.49044200	-1.91648300	-1.84620800
H	3.93437500	-0.17211600	-1.86970100
C	4.35277600	-3.62460000	0.46457600
C	3.25695000	-2.74032100	2.43595600
C	5.83585300	-0.49491500	1.94991500
C	4.98561700	1.40816600	0.71611700
P	-0.70103100	3.26809900	0.18647900
H	-2.49871400	-6.48166500	-2.73169200
H	-8.28124100	-0.25714400	1.03152500

C	5.98933500	-1.41018000	-2.70949200
C	4.47735500	-4.86151600	1.09491700
H	4.76864800	-3.46870400	-0.54085700
C	3.40070800	-3.97251100	3.06804600
H	2.75917300	-1.90926000	2.95501400
C	6.86193000	0.29957000	2.46126800
H	5.76622200	-1.55627000	2.22773500
C	6.02004500	2.19256600	1.22006400
H	4.24954500	1.84267900	0.02121300
C	0.15856700	3.23880100	1.80947000
C	-2.46228400	3.48528800	0.57155600
C	-0.15478700	4.90552500	-0.38512700
H	7.05746200	-1.68018700	-2.67107000
H	5.88462700	-0.38286900	-3.11961700
H	5.45641400	-2.11219300	-3.38760600
C	4.00451000	-5.03628900	2.39608300
H	4.95620000	-5.69582700	0.56576400
H	3.01969700	-4.10657700	4.08876200
C	6.95668500	1.64228200	2.09758400
H	7.59682600	-0.13828700	3.14959100
H	6.09367100	3.24799300	0.92600600
O	-0.05699600	4.41352500	2.53507400
H	-0.15100000	2.32737600	2.37037200
H	1.23776300	3.11800800	1.55428800
C	-3.39848800	3.39619500	-0.46725500
C	-2.90219200	3.73235100	1.87807200
C	-1.00406800	6.01322100	-0.37379000
C	1.17584500	5.05111200	-0.79907400
H	4.10673700	-6.01122000	2.89098500
H	7.76625700	2.26515600	2.50046300
C	0.82654300	4.48332300	3.63305900
C	-4.75626400	3.56338000	-0.20599400
H	-3.06963400	3.16943200	-1.49019000
C	-4.26385300	3.88401900	2.13670000
H	-2.16908500	3.82866700	2.69082700
C	-0.52698800	7.26118600	-0.77654500
H	-2.04535700	5.89910200	-0.04010300
C	1.65033200	6.30078700	-1.18898700
H	1.84379200	4.17563800	-0.83978000
H	0.60945500	5.42078500	4.17070000
H	1.88380800	4.48956400	3.29083100
H	0.69115400	3.61943600	4.31860600
C	-5.19180400	3.80662700	1.09809200
H	-5.47847200	3.48554100	-1.02923700
H	-4.60121400	4.06653000	3.16523000
C	0.79901400	7.40819200	-1.18119500

H	-1.20007800	8.12857600	-0.76918100
H	2.69297900	6.40735700	-1.51607300
H	-6.26245500	3.93854100	1.30647300
H	1.17220900	8.39099700	-1.49776000
C	0.88082000	-2.91638600	-1.08635300
Ir	0.27825100	-1.22873500	-1.66066200
O	1.31833100	-3.95731600	-0.78918000
C	-1.29256200	-1.60060800	-2.65066800
C	1.52393200	-0.78221500	-2.99964600
O	-2.22529900	-1.86009100	-3.29757000
O	2.23920900	-0.51509700	-3.88493400
C	-0.43494700	2.93933400	-2.67025900
H	-1.40270700	3.46203600	-2.64492300
H	0.43711900	3.60694200	-2.68879100
C	-0.33874600	1.66164600	-3.25822600
H	-1.24178000	1.16887900	-3.64659200
H	0.59944500	1.38554600	-3.75647800

Ir4(CO)9(PPh2CH2OPh)3

Ir	0.74788000	1.29629100	0.38537000
P	0.72760000	3.59811600	0.52345500
C	-0.88881100	0.90135700	1.57453300
C	-0.11089500	4.18171300	2.09067500
C	-0.02926700	4.53512000	-0.82972800
C	2.35736900	4.38767900	0.68701900
C	2.05455300	1.15135500	1.68243700
C	1.83931900	1.22502000	-1.38012600
Ir	-0.67829600	-0.96643200	0.68686000
O	-1.56664000	1.45714000	2.38802900
O	-0.72166000	5.44163200	2.00309400
H	0.71038400	4.25804800	2.83010900
H	-0.79370500	3.38564000	2.43756400
C	-1.41940900	4.55811700	-0.98929800
C	0.78721300	5.18466200	-1.76210800
C	3.54446800	3.71309100	0.39439400
C	2.40144800	5.72069800	1.12278600
O	2.85011400	0.98832300	2.52620300
O	2.49061100	1.92880600	-2.08130100
P	-2.78095400	-1.85242200	0.98502400
C	-0.11239400	-2.29083200	-0.80829200
C	-0.00155900	-1.84006500	2.16417400
C	-1.98766000	5.25222400	-2.05300500
H	-2.07707100	4.03749200	-0.27978900
C	0.21302600	5.86075000	-2.83764500
H	1.88020500	5.15495200	-1.65193200
C	4.76852800	4.36716700	0.53592000

H	3.52008800	2.67294500	0.03934800
C	3.62644800	6.36592800	1.26857000
H	1.46380600	6.25437600	1.34587300
C	-3.51625500	-2.43783400	-0.59160800
C	-4.03228500	-0.75094900	1.68355200
C	-2.84131000	-3.35674100	1.99897200
Ir	1.14213900	-0.74231700	-1.35477400
O	-0.37522700	-3.39629500	-1.18081400
O	0.42928500	-2.37064800	3.11629300
C	-1.17297700	5.90260600	-2.98135300
H	-3.08061900	5.27733600	-2.15474500
H	0.86025500	6.35514300	-3.57352600
C	4.81299700	5.68975400	0.97307900
H	5.69253200	3.82290300	0.29572800
H	3.65561900	7.40744300	1.61472200
O	-4.66667000	-3.19224200	-0.31278200
H	-3.74113400	-1.54824300	-1.22037200
H	-2.73627800	-3.03734500	-1.11092600
C	-5.21748800	-0.45258200	1.00122100
C	-3.76835300	-0.13853400	2.91457500
C	-3.81449900	-3.54065400	2.98391900
C	-1.90169300	-4.36292600	1.74507800
P	3.12215300	-1.67226100	-0.67039800
C	1.42740300	-1.17460800	-3.12488700
H	-1.62229900	6.43828700	-3.82784500
H	5.77827800	6.20088300	1.08612500
C	-6.11925300	0.46342400	1.53912500
H	-5.45425400	-0.95064700	0.05125500
C	-4.67645500	0.76962800	3.45299400
H	-2.83544900	-0.36156900	3.45028800
C	-3.83587500	-4.72133000	3.72579900
H	-4.56001500	-2.75407600	3.16837600
C	-1.93605800	-5.54484700	2.48016100
H	-1.14694800	-4.22426700	0.95482300
C	3.07550100	-2.35403700	1.03573000
C	4.49587200	-0.49316000	-0.64317200
C	3.73238100	-3.07512600	-1.63959800
O	1.57551200	-1.41543300	-4.25784800
C	-5.84826100	1.08029500	2.76098500
H	-7.04381200	0.69660700	0.99538600
H	-4.45498100	1.25370700	4.41301300
C	-2.89778400	-5.72278100	3.47671800
H	-4.59651500	-4.86020300	4.50526800
H	-1.20051000	-6.33351400	2.27509200
O	4.33248800	-2.90694900	1.32062900
H	2.79979500	-1.53889900	1.74092900

H	2.26405200	-3.11532700	1.06314100
C	4.88413300	0.07542200	-1.86344100
C	5.10819700	-0.07611300	0.54372200
C	5.10329800	-3.34921500	-1.70655100
C	2.81429100	-3.91931400	-2.27384100
H	-6.55993700	1.80274800	3.18302800
H	-2.91671500	-6.65134200	4.06223600
C	5.89021800	1.03625100	-1.89843500
H	4.38473900	-0.22808600	-2.79556900
C	6.10743000	0.89627700	0.50504200
H	4.82018200	-0.51388700	1.50880400
C	5.55258200	-4.45923500	-2.41772000
H	5.81802000	-2.68390000	-1.20185800
C	3.27104200	-5.03260200	-2.97696700
H	1.73513000	-3.70865600	-2.21501900
C	6.50392400	1.44808100	-0.71353200
H	6.18476400	1.47877800	-2.85851100
H	6.58192700	1.21914700	1.44101300
C	4.63795400	-5.30081800	-3.05336300
H	6.62845200	-4.66962200	-2.47691400
H	2.54890400	-5.69128700	-3.47640600
H	7.30221700	2.20250600	-0.74264000
H	4.99536800	-6.17311000	-3.61633300
C	-2.65461700	1.49128300	-0.61857200
Ir	-1.19708000	0.65850000	-1.47455100
O	-3.56930300	2.00850100	-0.10865000
C	-0.60424100	1.95348400	-2.72643400
C	-1.85484000	-0.67395100	-2.63288700
O	-0.26765000	2.72431000	-3.52821900
O	-2.24729000	-1.47598400	-3.38763900
C	4.52265100	-3.42280100	2.57114100
C	5.80215300	-3.92480600	2.82855900
C	3.53088700	-3.45966700	3.55350200
C	6.08993300	-4.46397700	4.07683900
H	6.55356200	-3.88047800	2.02933400
C	3.83896200	-4.00522100	4.80239400
H	2.52006300	-3.07377700	3.36519000
C	5.10982500	-4.50675700	5.07311300
H	7.09558600	-4.85679900	4.27584600
H	3.05969700	-4.03357100	5.57514800
H	5.33924300	-4.93149400	6.05830400
C	-2.08568100	5.51711800	1.90690700
C	-2.59426800	6.80598600	1.71913900
C	-2.95399700	4.42242000	1.97352200
C	-3.96530000	6.99894300	1.59146400
H	-1.88724900	7.64339800	1.65905300

C	-4.32806700	4.63314500	1.83645800
H	-2.60091600	3.39146000	2.11372400
C	-4.84419200	5.91305900	1.64672200
H	-4.35260100	8.01478500	1.43814900
H	-4.99161200	3.75647000	1.86715800
H	-5.92490700	6.06703300	1.53560100
C	-5.30447800	-3.74589400	-1.38544300
C	-6.43117600	-4.51961600	-1.08859800
C	-4.89144400	-3.56830800	-2.70888700
C	-7.14624600	-5.11656900	-2.11996300
H	-6.72048300	-4.64057400	-0.03653800
C	-5.62265000	-4.17718600	-3.73216800
H	-4.00719500	-2.96601200	-2.95810800
C	-6.74706700	-4.94896800	-3.44957500
H	-8.02875000	-5.72487800	-1.88234600
H	-5.29746300	-4.03894100	-4.77155400
H	-7.31275000	-5.42175200	-4.26206600

$Ir_4(CO)_8(C_2H_4)(PPh_2CH_2OPh)_3$
Apical.1.C_2H_4

Ir	-1.37898100	0.50647900	0.22042800
P	-3.65360500	0.14345300	0.19063800
C	-0.82408900	-1.10321200	1.42098500
C	-4.12696000	-0.56526200	1.82391300
C	-4.35059000	-1.00368100	-1.01777500
C	-4.70826100	1.61346500	0.02372500
C	-1.52259200	1.74305500	1.58413100
C	-1.35188600	1.70070400	-1.47741300
Ir	1.02870700	-0.59065500	0.65949700
O	-1.34189600	-1.85326900	2.19488700
O	-5.48006400	-0.93225200	1.89422000
H	-3.89837600	0.21851700	2.57710400
H	-3.42599600	-1.40077100	2.01077600
C	-4.54227100	-2.35559700	-0.71465900
C	-4.67014500	-0.51985400	-2.29282100
C	-4.17739400	2.90647700	-0.00508900
C	-6.09994100	1.43138500	-0.01656500
O	-1.53863300	2.50236100	2.47704300
O	-2.09811900	2.27508800	-2.20133200
P	2.20578500	-2.54381800	0.90177700
C	2.35446500	0.28290100	-0.66615200
C	1.66074500	0.14051900	2.24119800
C	-5.05776200	-3.21521500	-1.68245900
H	-4.29009900	-2.75861800	0.27728100
C	-5.17604800	-1.38658800	-3.25797000

H	-4.50606900	0.54024800	-2.53625100
C	-5.03044000	4.00706600	-0.06787400
H	-3.08914500	3.06415100	-0.00240300
C	-6.94617300	2.53517700	-0.07246700
H	-6.51598200	0.41375800	0.00139800
C	3.45466800	-2.78323500	-0.42487200
C	1.27378500	-4.09571700	0.91404300
C	3.29751400	-2.64254000	2.35378200
Ir	0.68628900	1.29963100	-1.31469800
O	3.52147600	0.23664300	-0.93835500
O	2.03890700	0.58105200	3.25947400
C	-5.37568400	-2.73393900	-2.95295000
H	-5.21215600	-4.27309100	-1.43367200
H	-5.40710900	-1.00450800	-4.26059700
C	-6.41228000	3.82521000	-0.09751300
H	-4.59519200	5.01523800	-0.10460800
H	-8.03385300	2.38777200	-0.09738800
O	4.23660400	-3.91237800	-0.12695600
H	2.92308200	-2.88907000	-1.39537200
H	4.06316600	-1.85269700	-0.47627900
C	1.46156400	-5.07756400	-0.06740600
C	0.31735600	-4.30160000	1.91664000
C	3.31034500	-3.74227400	3.21383000
C	4.19745500	-1.58947000	2.55685000
P	1.25550300	3.35800000	-0.46560500
C	1.21313300	1.68777500	-3.03393500
H	-5.78085300	-3.41486200	-3.71310500
H	-7.08147600	4.69455700	-0.14811700
C	0.68359500	-6.23346400	-0.06073600
H	2.24837500	-4.97158000	-0.82638200
C	-0.44968500	-5.46467600	1.92487100
H	0.15225400	-3.53590300	2.68600200
C	4.20784700	-3.78027500	4.28103300
H	2.61720500	-4.57846300	3.04338000
C	5.10124500	-1.63776500	3.61404000
H	4.19855400	-0.72462200	1.87474500
C	1.84114600	3.31158800	1.27731000
C	-0.10842700	4.54753700	-0.43600800
C	2.61144600	4.22985000	-1.29264200
O	1.52089400	1.87190900	-4.14746400
C	-0.27617300	-6.42831300	0.93148100
H	0.83802500	-6.99399800	-0.83730400
H	-1.20143200	-5.61061500	2.71179500
C	5.10324700	-2.73071800	4.48294400
H	4.20931100	-4.64404500	4.95884900
H	5.80713600	-0.81063800	3.76415100

O	2.22754300	4.61010000	1.64255200
H	1.03013400	2.90575700	1.92362000
H	2.69004300	2.59344800	1.31607400
C	-0.67229600	4.91832700	-1.66392700
C	-0.65593100	5.03830200	0.75444800
C	2.67840800	5.62776800	-1.27799500
C	3.63562600	3.48427400	-1.88670600
H	-0.88948200	-7.33891100	0.93269500
H	5.81071300	-2.76464900	5.32174400
C	-1.75551600	5.79081400	-1.70210800
H	-0.26238700	4.51071400	-2.59991100
C	-1.75015800	5.90243000	0.71270900
H	-0.22581100	4.76543800	1.72750000
C	3.76055600	6.27532000	-1.87002200
H	1.87539300	6.20818000	-0.80202000
C	4.72079000	4.13897500	-2.46691400
H	3.59164000	2.38405200	-1.88490800
C	-2.29607500	6.28515400	-0.51299700
H	-2.19164200	6.07329000	-2.66874600
H	-2.17174800	6.28509600	1.65137500
C	4.78221200	5.53253500	-2.46419800
H	3.80819600	7.37222000	-1.86536600
H	5.52306100	3.55117800	-2.93153300
H	-3.14640100	6.98043000	-0.54356100
H	5.63335200	6.04570300	-2.93092400
C	-1.21317300	-2.65006700	-0.84310200
Ir	-0.34524900	-1.19749800	-1.66939200
O	-1.75266000	-3.57453800	-0.37890100
C	-1.44411700	-0.68740800	-3.09862300
O	-2.13907500	-0.37273400	-3.98274900
C	1.38224300	-1.55870700	-3.01418700
H	1.23202500	-1.04017800	-3.96976200
H	2.34766600	-1.34408700	-2.53632100
C	0.71455800	-2.77977100	-2.77807400
H	0.04562000	-3.20034500	-3.53909400
H	1.13944300	-3.52206100	-2.08426400
C	2.67512100	4.80046000	2.91812100
C	3.02716300	6.11318100	3.24821300
C	2.78389000	3.77536400	3.86008700
C	3.49159200	6.39912300	4.52667700
H	2.92806600	6.89081500	2.47941800
C	3.25294700	4.08144900	5.14010000
H	2.51663700	2.73932000	3.61232300
C	3.60864300	5.38425100	5.48166100
H	3.76973600	7.43026200	4.78113400
H	3.33968800	3.27509000	5.88018400

H	3.97753000	5.61092800	6.48975600
C	5.15248500	-4.29164700	-1.06194400
C	5.38114600	-3.59600200	-2.25252200
C	5.87408600	-5.45341400	-0.76982300
C	6.33802200	-4.07889000	-3.14903200
H	4.83093700	-2.67481800	-2.48502600
C	6.82260900	-5.91936300	-1.67188200
H	5.67036400	-5.96969500	0.17748300
C	7.05959200	-5.23695100	-2.86939500
H	6.51804500	-3.53002200	-4.08258900
H	7.38693900	-6.83116000	-1.43683300
H	7.80957300	-5.60689600	-3.57943900
C	-5.81475500	-2.17950900	2.33891100
C	-7.15888800	-2.53114300	2.16360200
C	-4.92595200	-3.08430400	2.93028600
C	-7.61110700	-3.78100100	2.56923200
H	-7.83029900	-1.79991900	1.69382100
C	-5.39762000	-4.33825600	3.32767700
H	-3.87077100	-2.83328700	3.10274000
C	-6.73203100	-4.69739100	3.15287600
H	-8.66702200	-4.04476700	2.42446600
H	-4.69596400	-5.04383000	3.79223300
H	-7.08763500	-5.68512300	3.47118500

$Ir_4(CO)_8(C_2H_4)(PPh_2CH_2OPh)_3$
Apical.2.C_2H_4

Ir	-1.41859700	0.43570700	0.18166500
P	-3.65724300	-0.05413700	0.10532900
C	-0.80618900	-1.21742400	1.26395200
C	-4.12259200	-0.84173800	1.69752400
C	-4.24638800	-1.25084700	-1.11922800
C	-4.80613300	1.33929200	-0.07536400
C	-1.62545400	1.61206500	1.59485800
C	-1.42505200	1.70016900	-1.44719900
Ir	1.04765400	-0.54217900	0.61950000
O	-1.28535800	-2.06611700	1.95931200
O	-5.46269100	-1.26176300	1.69728500
H	-3.92771100	-0.10672900	2.50734300
H	-3.39963400	-1.67224900	1.83562800
C	-4.37914800	-2.60989800	-0.80409800
C	-4.53670000	-0.80638600	-2.41516700
C	-4.35581700	2.66239900	-0.03924100
C	-6.17739500	1.07251200	-0.20480100
O	-1.68703700	2.32984200	2.51952100
O	-2.17053500	2.31715500	-2.13570400
P	2.33708700	-2.40930900	0.96995000

C	2.36109100	0.38115700	-0.69444700
C	1.61854400	0.17098400	2.22487900
C	-4.79055000	-3.51338800	-1.78276000
H	-4.19609700	-2.97855200	0.21692300
C	-4.94336600	-1.71463600	-3.38942000
H	-4.43572100	0.25977600	-2.66571700
C	-5.26970000	3.71128700	-0.12521200
H	-3.28149800	2.88141200	0.03451000
C	-7.08495700	2.12463100	-0.28569100
H	-6.52698200	0.03096900	-0.23843400
C	3.16659400	-3.01169400	-0.55243600
C	1.49530500	-3.86520600	1.63265200
C	3.75829800	-2.17615500	2.07845900
Ir	0.64074200	1.32941100	-1.33333000
O	3.52775200	0.37613700	-0.95714500
O	1.94933100	0.59319300	3.26775500
C	-5.07048400	-3.06935500	-3.07574000
H	-4.90031200	-4.57483200	-1.52536400
H	-5.15378600	-1.35920000	-4.40623600
C	-6.63251200	3.44544200	-0.24561600
H	-4.89736500	4.74495700	-0.10861700
H	-8.15807900	1.91312800	-0.38158600
O	4.09592500	-4.00904200	-0.22239800
H	2.38388300	-3.38706400	-1.24813500
H	3.64889500	-2.12837400	-1.02595600
C	1.52337300	-5.10749600	0.98741500
C	0.79201800	-3.72183000	2.83443700
C	4.10556300	-3.12974500	3.03910300
C	4.54423900	-1.02881400	1.91578000
P	1.12004700	3.38242700	-0.42021000
C	1.11576900	1.83431400	-3.04329400
H	-5.39307600	-3.78392800	-3.84427800
H	-7.35150400	4.27253900	-0.31626900
C	0.84688000	-6.19383500	1.54143800
H	2.10558000	-5.23929000	0.06458000
C	0.13540200	-4.81420800	3.39379600
H	0.75701900	-2.74324700	3.33397400
C	5.22394200	-2.92674700	3.84657500
H	3.49623100	-4.03685700	3.15707400
C	5.66629800	-0.83723000	2.71785900
H	4.28468600	-0.28967100	1.14158300
C	1.67198200	3.31616400	1.33257300
C	-0.29312400	4.51233300	-0.38023900
C	2.44539500	4.33027400	-1.21372200
O	1.38796300	2.12313600	-4.14184200
C	0.15636700	-6.05003800	2.74527500

H	0.86982000	-7.16501100	1.03018000
H	-0.40907400	-4.69367800	4.33944600
C	6.00407500	-1.78155900	3.68893700
H	5.48903900	-3.67427700	4.60579000
H	6.28108700	0.06236000	2.58436700
O	1.99610100	4.62061900	1.73604400
H	0.86194600	2.86442600	1.94996700
H	2.54995900	2.63418300	1.37412100
C	-0.83456000	4.91798300	-1.60709300
C	-0.90703500	4.90646700	0.81335800
C	2.45693900	5.72853600	-1.14675900
C	3.49130200	3.64882600	-1.84573900
H	-0.36891200	-6.90963900	3.18187100
H	6.88454400	-1.62405600	4.32562000
C	-1.96480600	5.72907200	-1.63860900
H	-0.37343200	4.58394300	-2.54853600
C	-2.04861400	5.70740600	0.77713000
H	-0.49304700	4.60495000	1.78511300
C	3.50699400	6.44082600	-1.72140800
H	1.63439300	6.25639000	-0.64386900
C	4.54291100	4.36811200	-2.41112200
H	3.48830900	2.54893900	-1.89240000
C	-2.57514200	6.12389900	-0.44588200
H	-2.38348000	6.03845800	-2.60474200
H	-2.52442000	6.01165300	1.71860000
C	4.55021000	5.76180900	-2.35367200
H	3.51111500	7.53779600	-1.67547900
H	5.36013600	3.83067800	-2.90930400
H	-3.46549900	6.76719900	-0.47083300
H	5.37510500	6.32560200	-2.80903700
Ir	-0.25420600	-1.18861900	-1.74913600
C	-1.40985900	-0.52798500	-3.07497300
C	1.33577100	-1.59409500	-2.63431800
O	-2.06613200	-0.14359600	-3.95981800
O	2.29975900	-1.73905900	-3.28869400
C	2.41502000	4.79283900	3.02544400
C	2.71820900	6.10700900	3.39444800
C	2.54428700	3.74763700	3.94257000
C	3.15003200	6.37476800	4.68834300
H	2.60749900	6.90062900	2.64342200
C	2.98057900	4.03500600	5.23790200
H	2.31755900	2.71064500	3.66289100
C	3.28411000	5.34003800	5.61910500
H	3.38712600	7.40773700	4.97479200
H	3.08594600	3.21229000	5.95711300
H	3.62786200	5.55304400	6.63897400

C	-5.77795700	-2.41549700	2.35345200
C	-7.09247800	-2.86314600	2.17527600
C	-4.89079500	-3.14057600	3.15630900
C	-7.51800200	-4.03121400	2.79505800
H	-7.76059300	-2.27064800	1.53641700
C	-5.33521400	-4.31657600	3.76725200
H	-3.86256700	-2.79965800	3.33370800
C	-6.64040300	-4.76957900	3.59503300
H	-8.55085900	-4.37344500	2.64898700
H	-4.63748800	-4.88160200	4.39926300
H	-6.97626900	-5.69268000	4.08339200
C	4.83345700	-4.52014200	-1.24992700
C	5.75480600	-5.51199000	-0.89791500
C	4.70114100	-4.10791100	-2.57911700
C	6.54692300	-6.09305600	-1.88148600
H	5.83606400	-5.80174800	0.15766000
C	5.50664100	-4.70457800	-3.55261900
H	3.98928700	-3.32201100	-2.86927300
C	6.42680500	-5.69489700	-3.21623800
H	7.27103800	-6.86934600	-1.60168600
H	5.40519400	-4.38042300	-4.59650700
H	7.05138600	-6.15699500	-3.99096500
C	-1.03657300	-3.06861300	-0.87678500
H	-0.25290300	-3.62638800	-0.34510300
H	-1.94284800	-2.87074100	-0.29053800
C	-1.15243700	-3.14000400	-2.27780000
H	-2.14463200	-3.01129200	-2.73478300
H	-0.43959600	-3.73248400	-2.86631500

$Ir_4(CO)_8(C_2H_4)(PPh_2CH_2OPh)_3$
Axial.C_2H_4

Ir	1.32371100	0.98540700	-0.56834000
P	3.60218600	1.24539300	-0.61531800
C	1.16900700	-0.80175000	-1.54088600
C	4.35386000	0.30490100	-2.05045200
C	4.58437000	0.77463500	0.83483200
C	4.22085500	2.92933600	-0.94420600
C	1.13838100	2.25473200	1.00555600
Ir	-0.74163000	-0.73829500	-0.67947500
O	1.80735100	-1.50746600	-2.26975500
O	5.66865000	-0.14069700	-1.84805300
H	4.37563400	1.03181800	-2.88593300
H	3.65008100	-0.50059200	-2.33092800
C	4.82419800	-0.57292900	1.12719100
C	5.05745700	1.76579200	1.70190300
C	3.38923200	4.04533700	-0.82990300

C	5.55759700	3.09477500	-1.33227500
O	1.73660500	3.05092000	1.66112900
P	-1.39286300	-2.93794200	-0.84290900
C	-2.07058200	-0.26167700	0.82811000
C	-1.67474800	-0.30413900	-2.20695300
C	5.55219800	-0.92260800	2.26050100
H	4.45030200	-1.36895300	0.46744700
C	5.76805000	1.40904300	2.84704000
H	4.86021400	2.82528500	1.48735100
C	3.88663000	5.31963600	-1.10014700
H	2.34490700	3.91380200	-0.51418400
C	6.05115300	4.36939800	-1.60145400
H	6.21407900	2.21416600	-1.41665100
C	-1.82370800	-3.66807000	0.78178900
C	-0.18707900	-4.08407400	-1.54607500
C	-2.92626600	-3.17575700	-1.78784300
Ir	-0.73977600	1.26741300	1.18873800
O	-3.11129800	-0.65181500	1.27921000
O	-2.23919200	-0.02729100	-3.19898900
C	6.02275100	0.06702600	3.12537200
H	5.74795600	-1.98315800	2.46672300
H	6.12018400	2.19198500	3.53105400
C	5.21697900	5.48427600	-1.48493600
H	3.21994600	6.18889700	-1.00993700
H	7.09865500	4.49487000	-1.90567500
O	-2.42034400	-4.92336300	0.58216700
H	-0.89077000	-3.74079000	1.38234900
H	-2.50567800	-2.95298100	1.29267700
C	0.30431900	-5.18021200	-0.82718800
C	0.32509800	-3.80412600	-2.81866900
C	-3.06330400	-4.18607900	-2.74234700
C	-3.99294500	-2.30313600	-1.53580300
P	-2.20031900	2.87609400	0.44579200
C	-1.06598500	1.67196500	2.95707200
H	6.58535100	-0.21119700	4.02618900
H	5.60942500	6.48723500	-1.69863100
C	1.30434200	-5.98092300	-1.37634600
H	-0.10535000	-5.42927800	0.16107300
C	1.31048000	-4.61749400	-3.37136900
H	-0.04120700	-2.92928000	-3.37425300
C	-4.25727200	-4.31101200	-3.45331800
H	-2.22850500	-4.87606000	-2.93179800
C	-5.18559300	-2.43703700	-2.24165200
H	-3.89290500	-1.51873100	-0.76846600
C	-3.24236200	2.23809300	-0.93335000
C	-1.48822000	4.41390800	-0.19443500

C	-3.46249500	3.39371300	1.63957000
O	-1.23149600	1.88432700	4.09350200
C	1.80976500	-5.70088300	-2.64651800
H	1.68941900	-6.83502200	-0.80432400
H	1.71061300	-4.38585700	-4.36688200
C	-5.31671200	-3.43755700	-3.20717000
H	-4.35958700	-5.10154800	-4.20834900
H	-6.01611600	-1.74705600	-2.03573600
O	-4.34230900	3.08216800	-1.15642300
H	-2.60898400	2.12680300	-1.84118400
H	-3.56937500	1.22146400	-0.62430100
C	-0.45364300	5.02079700	0.53006700
C	-1.89155200	4.95695700	-1.42025000
C	-3.83088300	4.73474200	1.77445600
C	-4.09666200	2.40799500	2.40570800
H	2.59739300	-6.33349000	-3.07735800
H	-6.25414300	-3.53951600	-3.76995500
C	0.18753600	6.14723100	0.01821000
H	-0.12661100	4.59396500	1.48853300
C	-1.24132500	6.08026400	-1.93053800
H	-2.72852600	4.50710300	-1.97353000
C	-4.82684200	5.09179500	2.68248500
H	-3.33228000	5.50335500	1.16661300
C	-5.09949500	2.77102900	3.30110500
H	-3.80679100	1.34993500	2.30150900
C	-0.19712900	6.67158800	-1.21810700
H	1.00159400	6.61209700	0.59109400
H	-1.55379800	6.49617300	-2.89725400
C	-5.46231100	4.11143500	3.44462100
H	-5.10852800	6.14691500	2.79541300
H	-5.59650700	1.99696500	3.90001400
H	0.31698300	7.55144300	-1.62733700
H	-6.24581300	4.39437000	4.15984400
C	1.98617500	-2.25831200	0.77345900
Ir	0.96265400	-0.83160200	1.46908700
O	2.59950400	-3.17160900	0.38286400
C	2.09936800	0.06466400	2.69948300
C	-0.24186600	-1.61914100	2.67631700
O	2.75283500	0.59029600	3.50297400
O	-0.97203900	-2.10021900	3.45158600
C	1.58609500	1.82232600	-2.56618400
H	2.49110900	2.43023300	-2.71620500
H	1.42119700	1.04938400	-3.33045500
C	0.47420800	2.42358600	-1.93276600
H	-0.54098700	2.12399300	-2.22866300
H	0.55430500	3.45614100	-1.56274600

C	-5.35687700	2.56563200	-1.91430200
C	-6.54498700	3.30221300	-1.92478000
C	-5.24642500	1.38166900	-2.64874400
C	-7.62771500	2.84833800	-2.66930800
H	-6.59682900	4.22099000	-1.32607600
C	-6.34620000	0.93914100	-3.38833200
H	-4.30956100	0.80906700	-2.68125100
C	-7.53689900	1.66204400	-3.40404300
H	-8.56096300	3.42647400	-2.67056900
H	-6.25103500	0.01260500	-3.97159300
H	-8.39399800	1.30603900	-3.98922000
C	-2.80000700	-5.59979300	1.70527700
C	-2.63837200	-5.10263300	3.00164200
C	-3.37213300	-6.85799500	1.49120500
C	-3.05907400	-5.88338700	4.08151600
H	-2.19500300	-4.11452500	3.18540800
C	-3.78345200	-7.62049700	2.57785800
H	-3.48477800	-7.21193700	0.45817800
C	-3.62938200	-7.13822400	3.88130200
H	-2.93403800	-5.49240800	5.09971300
H	-4.23259500	-8.60727100	2.40505500
H	-3.95496200	-7.74144500	4.73791300
C	5.90466600	-1.47504200	-1.65464500
C	7.23749600	-1.80544900	-1.38996200
C	4.92741500	-2.47498700	-1.69367700
C	7.59209400	-3.13052400	-1.16308900
H	7.97846700	-0.99658100	-1.35168700
C	5.29999600	-3.80020600	-1.45614500
H	3.86715200	-2.26251900	-1.88938400
C	6.62504800	-4.13994300	-1.19308100
H	8.64084600	-3.37719300	-0.95150300
H	4.51415600	-4.56918100	-1.46888900
H	6.90536300	-5.18371700	-1.00363000

$Ir_4(CO)_8(C_2H_4)(PPh_2CH_2OPh)_3$
Equatorial.C_2H_4

Ir	-1.30003900	0.99302900	0.35671700
P	-3.58317700	1.18496600	0.50649100
C	-1.05192900	-0.69574800	1.50222900
C	-4.20880200	0.43793300	2.10099600
C	-4.60927200	0.49078900	-0.81631200
C	-4.21531200	2.88444900	0.64421700
C	-1.08023500	2.24522400	1.69338800
C	-1.04026700	2.12386300	-1.43858700
Ir	0.81951500	-0.70515000	0.60933400
O	-1.65594400	-1.32496300	2.32249900

O	-5.53023300	-0.03449800	2.06974000
H	-4.16682300	1.27384600	2.82758900
H	-3.47919100	-0.32301600	2.43314900
C	-4.80178200	-0.89107200	-0.92338900
C	-5.16062300	1.34511400	-1.77777900
C	-3.41121400	3.99273300	0.37296300
C	-5.54472800	3.06820700	1.05186200
O	-0.89276200	2.99427100	2.57479100
O	-1.69346300	2.80793900	-2.16587900
P	1.46866900	-2.88331400	0.83513500
C	2.16046900	-0.21473500	-1.01212400
C	1.72302800	-0.34835300	2.17417800
C	-5.55975400	-1.40975800	-1.96882900
H	-4.36870200	-1.58218200	-0.18651800
C	-5.90584000	0.81850600	-2.83154500
H	-4.99730200	2.42960100	-1.70751200
C	-3.93039600	5.28006000	0.51041600
H	-2.37233800	3.84994700	0.04229500
C	-6.05763300	4.35517800	1.18914400
H	-6.17692600	2.19112000	1.26134800
C	1.82005300	-3.71761100	-0.75749400
C	0.29409700	-3.97126000	1.67391200
C	3.04536400	-3.09597000	1.71178300
Ir	0.77532800	1.22022600	-1.28626300
O	3.15211700	-0.69399000	-1.48486700
O	2.24163000	-0.19493900	3.21695100
C	-6.11182500	-0.55705300	-2.92652900
H	-5.71635800	-2.49471600	-2.03137000
H	-6.32328000	1.49379700	-3.58955500
C	-5.25075400	5.46357100	0.91796700
H	-3.28249800	6.14270300	0.30023400
H	-7.09732100	4.49591900	1.51276900
O	2.41808300	-4.96016900	-0.49455700
H	0.85935300	-3.82155900	-1.30641900
H	2.48330600	-3.04099300	-1.34126000
C	-0.23330100	-5.11557600	1.06470700
C	-0.15253800	-3.59264000	2.94572100
C	3.21869100	-4.05959500	2.70707800
C	4.11109500	-2.26264400	1.34944500
P	1.90935600	2.92672000	-0.20158600
H	-6.70109800	-0.96925900	-3.75616200
H	-5.65772700	6.47747500	1.02872000
C	-1.20485400	-5.86789600	1.72267200
H	0.12577400	-5.43569100	0.07698000
C	-1.11118600	-4.35584400	3.60627700
H	0.24272600	-2.68110300	3.41688900

C	4.45110700	-4.17868300	3.34987500
H	2.38144600	-4.71681600	2.98227400
C	5.34270700	-2.39478400	1.98530400
H	3.97481200	-1.51196300	0.55474800
C	2.50464300	2.44441000	1.48406100
C	0.97237500	4.45736400	0.07315500
C	3.50104400	3.48041500	-0.88431600
C	-1.64666800	-5.48866500	2.99114300
H	-1.61974800	-6.76077300	1.23724500
H	-1.46157400	-4.04661600	4.59943600
C	5.51289100	-3.34835000	2.99145900
H	4.58234700	-4.93038600	4.13923400
H	6.17698600	-1.74418700	1.68761300
O	3.43920500	3.36707500	1.98938100
H	1.64080100	2.34249600	2.17099800
H	2.95360000	1.44345400	1.34799000
C	0.17470600	4.97141400	-0.95691000
C	1.02575300	5.12719600	1.30257400
C	3.79265400	4.83313500	-1.06958400
C	4.47503600	2.51069800	-1.15915800
H	-2.41223400	-6.08324900	3.50771400
H	6.48161200	-3.44649300	3.49906700
C	-0.56519200	6.13583900	-0.75940700
H	0.10804000	4.44708100	-1.91928300
C	0.27762000	6.28690900	1.49836800
H	1.66480500	4.75102600	2.11313800
C	5.05403300	5.21620500	-1.52911300
H	3.02847500	5.59209700	-0.84733500
C	5.73575900	2.89942100	-1.60395500
H	4.24540500	1.43989300	-1.03977700
C	-0.51846300	6.79361200	0.47081700
H	-1.19105000	6.52244100	-1.57473400
H	0.31665300	6.79718200	2.46939000
C	6.02727500	4.25226500	-1.79073400
H	5.27738700	6.28066700	-1.68007000
H	6.49766200	2.13558100	-1.80584600
H	-1.10413300	7.70932000	0.62960700
H	7.02065900	4.55594400	-2.14615700
C	-1.85693700	-2.32703000	-0.69501100
Ir	-0.86631100	-0.96665200	-1.53961700
O	-2.46146200	-3.19258600	-0.19544700
C	-2.09655500	-0.20371200	-2.76353300
C	0.32727300	-1.82228700	-2.71745400
O	-2.82403700	0.22643300	-3.56258400
O	1.02740600	-2.32448700	-3.50972100
C	4.73851200	2.93701600	2.09669800

C	5.73494300	3.86737200	1.80059700
C	5.06988400	1.64348300	2.51142900
C	7.07254900	3.49537600	1.89963500
H	5.43709900	4.86787000	1.45997600
C	6.41529700	1.28551700	2.60203700
H	4.29103700	0.92241000	2.80247100
C	7.42142300	2.20128800	2.29286000
H	7.85393800	4.22554700	1.65084900
H	6.67239400	0.27238400	2.94195700
H	8.47685200	1.90982400	2.36538600
C	-5.75595000	-1.38448400	2.06692600
C	-7.10320500	-1.75769400	2.03443200
C	-4.75667000	-2.36405000	2.08434300
C	-7.45002300	-3.10411800	2.01703800
H	-7.86451000	-0.96721500	2.01445000
C	-5.12269500	-3.71197300	2.06174000
H	-3.68545700	-2.11960200	2.10785600
C	-6.46222200	-4.09336400	2.02939900
H	-8.51112700	-3.38487800	1.98913100
H	-4.32161500	-4.46568800	2.05897000
H	-6.73922000	-5.15489900	2.00893700
C	2.73020300	-5.73080300	-1.57639000
C	3.28626200	-6.98163700	-1.28886900
C	2.51784800	-5.33330200	-2.89927700
C	3.62949300	-7.83699400	-2.32904600
H	3.44024100	-7.25603500	-0.23713300
C	2.87004400	-6.20663000	-3.93169700
H	2.08980900	-4.35065900	-3.13962200
C	3.42271300	-7.45556900	-3.65837300
H	4.06564100	-8.81788600	-2.09893800
H	2.70521200	-5.89393600	-4.97107700
H	3.69392000	-8.13252600	-4.47803200
C	1.64980400	2.25960800	-3.00379800
H	2.74700200	2.23037400	-2.98448500
H	1.21678400	3.25989600	-3.15482800
C	0.93293900	1.12601300	-3.43920600
H	-0.05136600	1.25758500	-3.90970700
H	1.49224500	0.23496600	-3.75536900